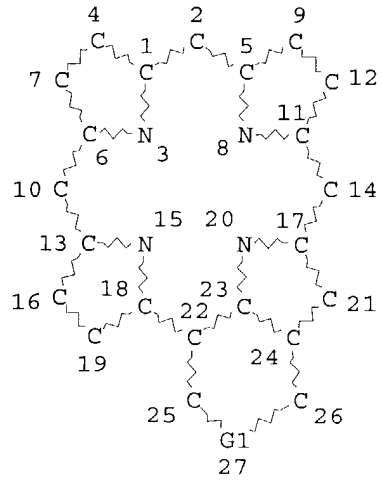
=> d que l18
L4 STR



REP G1=(0-10) A
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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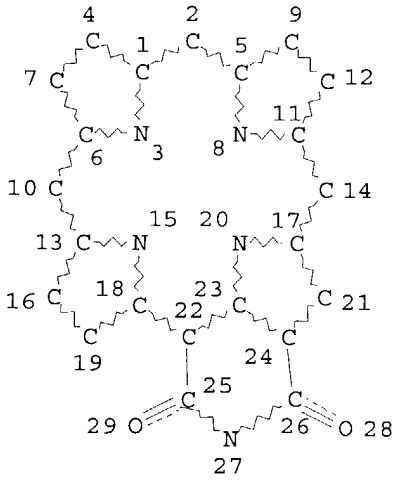
L12 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1

NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE
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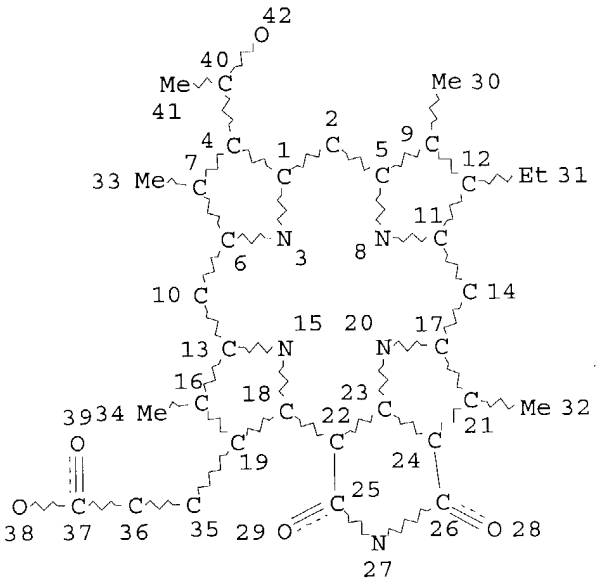
L14 18 SEA FILE=REGISTRY ABB=ON PLU=ON L13 AND C6/ES AND F>5
L16 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 4
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L17 86 SEA FILE=REGISTRY SUB=L6 SSS FUL L16
L18 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 OR L14

=> d l18 ibib ab hitstr 1-21

L18 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:236230 HCAPLUS
DOCUMENT NUMBER: 141:38481
TITLE: Method for the preparation of hydrazides of bacteriochlorophyll a eliciting photodynamic activity
INVENTOR(S): Mironov, A. F.; Grin, M. A.; Tsiprovskii, A. G.; Dzardanov, D. V.; Golovin, K. V.; Feofanov, A. V.; Karmakova, T. A.; Yakubovskaya, R. I.
PATENT ASSIGNEE(S): Russia
SOURCE: Russ., No pp. given
CODEN: RUXXE7
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RU 2223274	C1	20040210	RU 2002-123618	20020904
PRIORITY APPLN. INFO.:			RU 2002-123618	20020904

OTHER SOURCE(S): CASREACT 141:38481; MARPAT 141:38481

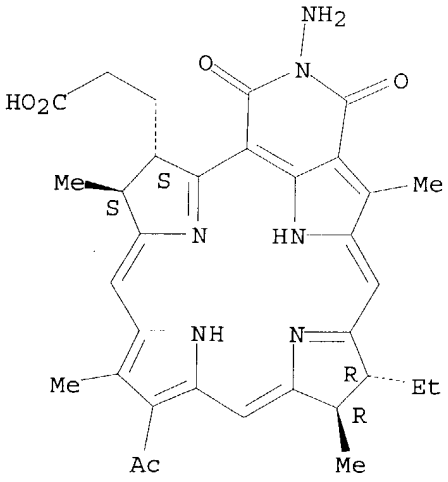
AB Invention relates to bacteriochlorophyll a hydrazides I [R1 = COCH3, CH(OH)CH3, CH:CH2; R2 = H, CH3, C2H5; R3, R4 = H, CH3, Tosyl] and a method for their preparation The method for preparing hydrazides I involves interaction of derivs. of bacteriochlorophyll a containing a cyclic anhydride with hydrazine hydrate and the following cyclization of formed intermediate hydrazide by addition of hydrochloric acid to reaction mass. Thus, bacteriopurpurin in pyridine was treated with NH2NH2 in pyridine, cyclized with aqueous HCl, esterified with CH2N2 in Et2O, alkylateds with MeI to give I (R1 = COMe, R2 = R3 = R4 = Me). Proposed hydrazides show high photoinduced activity. In the absence of light irradiation hydrazides I in concentration 6-15 times exceeding phototoxic doses do not have an effect on cellular culture growth [I (R1 = COMe, R2 = R3 = R4 = Me) gave IC50 = 0.19 μm/L and IC50 = 0.4 μm/L].

IT **700862-74-4P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of; preparation of hydrazides of bacteriochlorophyll a eliciting photodynamic activity)

RN 700862-74-4 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-amino-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

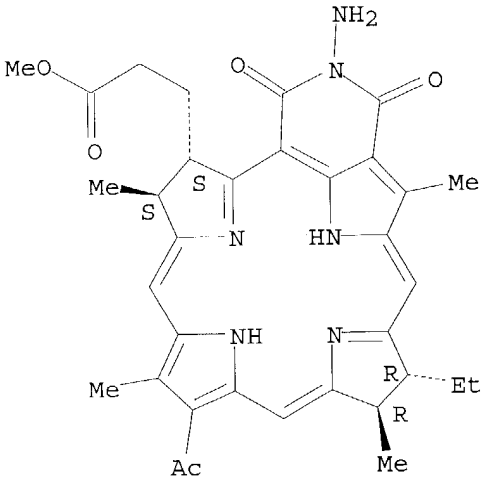
Absolute stereochemistry.



IT **700817-29-4P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation or tosylation of; preparation of hydrazides of bacteriochlorophyll a eliciting photodynamic activity)

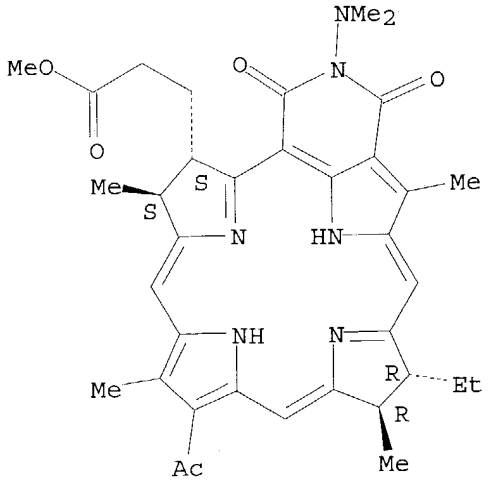
RN 700817-29-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-amino-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **700817-30-7P 700817-31-8P 700817-33-0P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of hydrazides of bacteriochlorophyll a eliciting photodynamic activity)
RN 700817-30-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-(dimethylamino)-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

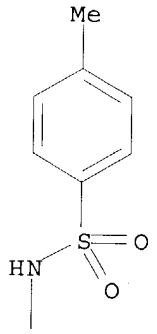
Absolute stereochemistry.



RN 700817-31-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-19-[[(4-methylphenyl)sulfonyl]amino]-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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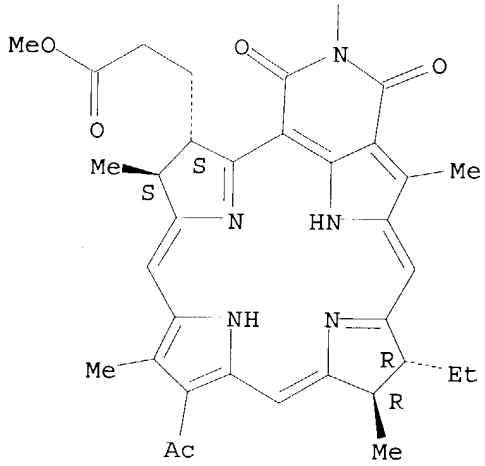
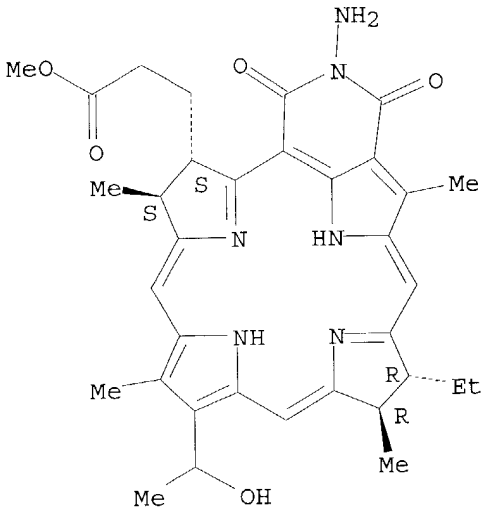


RN 700817-33-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-amino-5-ethyl-1,5,6,15,16,18,19,20-octahydro-10-(2-hydroxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:145474 HCAPLUS
DOCUMENT NUMBER: 141:23326
TITLE: Synthesis of derivatives of purpurin-18 imide and research on the visible spectra
AUTHOR(S): Han, Guang-Fan; Wang, Jin-Jun; Chang, Xiu-Juan
CORPORATE SOURCE: School of Material and Engineering, East China Shipbuilding Institute, Zhenjiang, 212003, Peop. Rep. China
SOURCE: Youji Huaxue (2004), 24(2), 187-194
CODEN: YCHHDX; ISSN: 0253-2786
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 141:23326

AB Me pheophorbide-a was used as a starting material for modifications at 3-position and transformation on E-ring. The introduction of biphenyloxy was performed by addition of HBr and nucleophilic substitution with phenylphenol on vinyl group at 3-position. In basic condition E-ring was converted into the cyclohexanedicarboxylic anhydride to form purpurin-18 derivs. by the air-oxidation The oxidized products were reacted with hydroxyamine hydrochloride to generate purpurin-18 imide by ammonolysis and recondensation. The alkylation and acylation for hydroxy group linked with nitrogen were accomplished to give N-alkoxy and N-acyloxy purpurin-18 imides, resp. The effect on their visible spectra by variation of chemical construction was discussed. The structures of all new compds. were characterized by elemental anal., UV, IR and 1H NMR spectra.

IT **698392-28-8P 698392-29-9P 698392-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

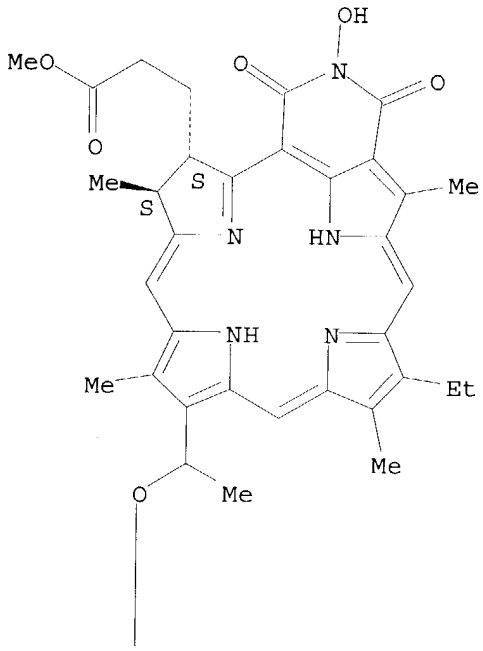
(of hydroxyl group linked with nitrogen)

RN 698392-28-8 HCAPLUS

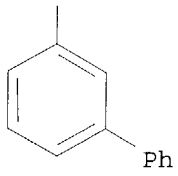
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-3-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-19-hydroxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

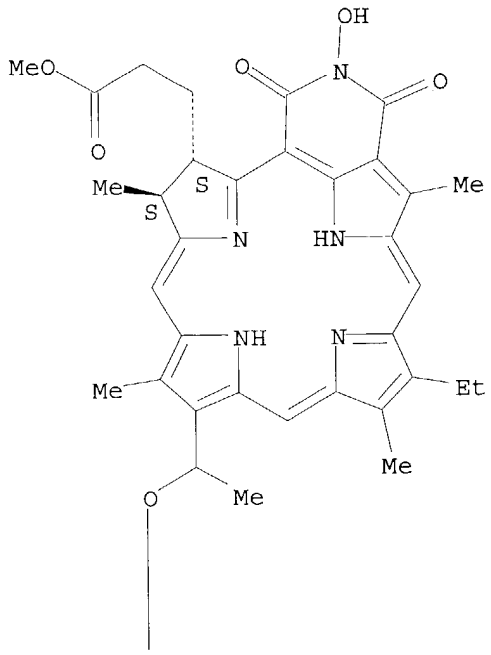


RN 698392-29-9 HCAPLUS

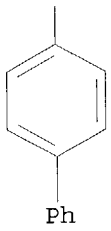
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-4-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-19-hydroxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



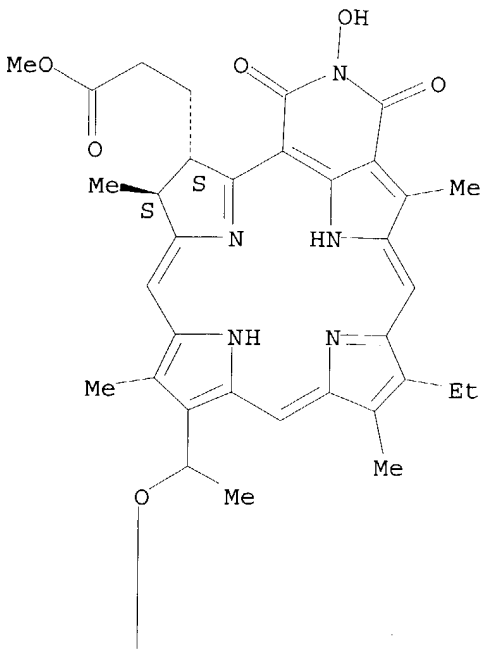
PAGE 2-A



RN 698392-30-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-2-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-19-hydroxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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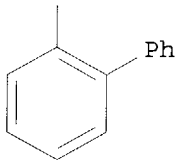


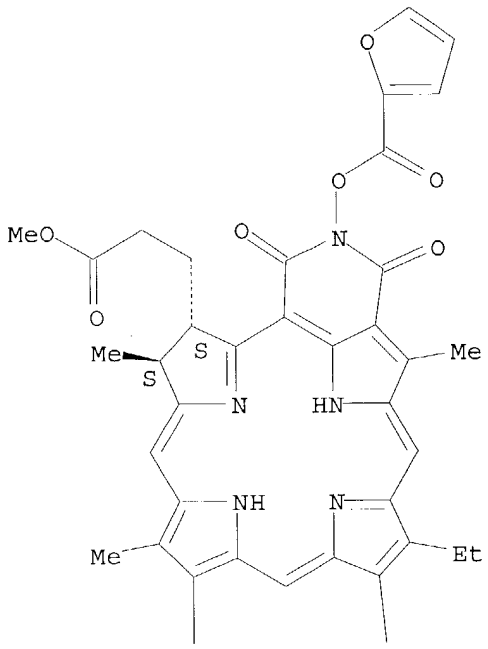
IT **698392-31-3P 698392-32-4P 698392-33-5P**
698392-34-6P 698392-35-7P 698392-36-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(of hydroxyl group linked with nitrogen)

RN 698392-31-3 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-3-yloxy)ethyl]-5-ethyl-19-[(2-furanylcarbonyl)oxy]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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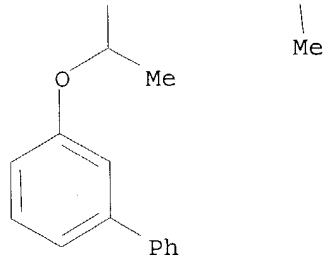
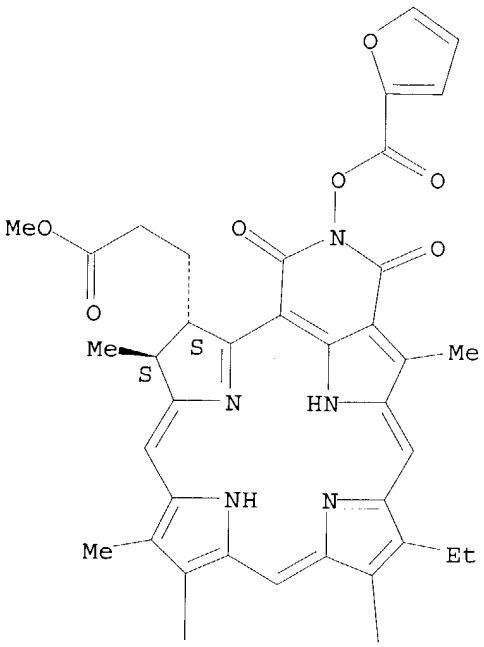


RN 698392-32-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-2-yloxy)ethyl]-5-ethyl-19-[(2-furanylcarbonyl)oxy]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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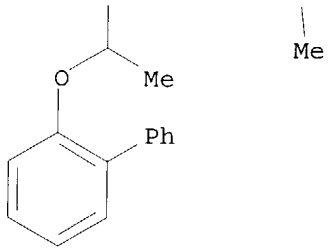
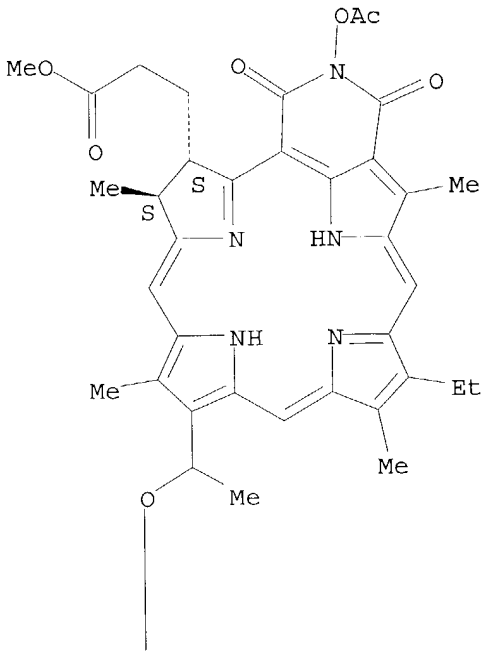


RN 698392-33-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-(acetyloxy)-10-[1-([1,1'-biphenyl]-3-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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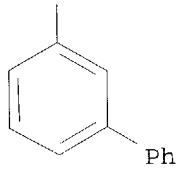
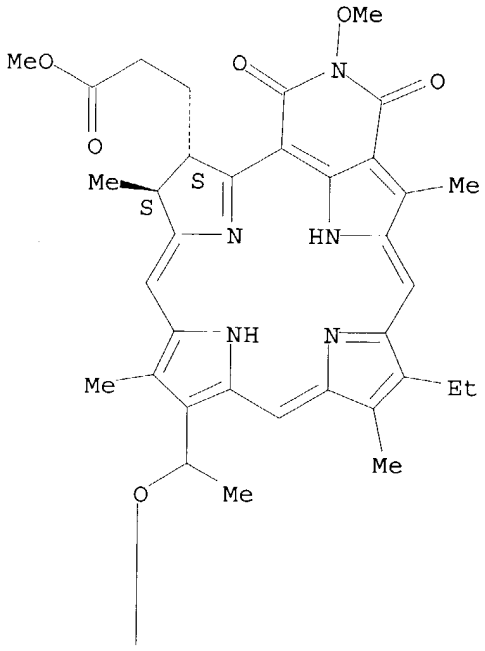


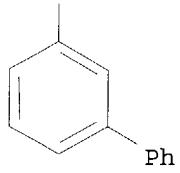
RN 698392-34-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-3-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-19-methoxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



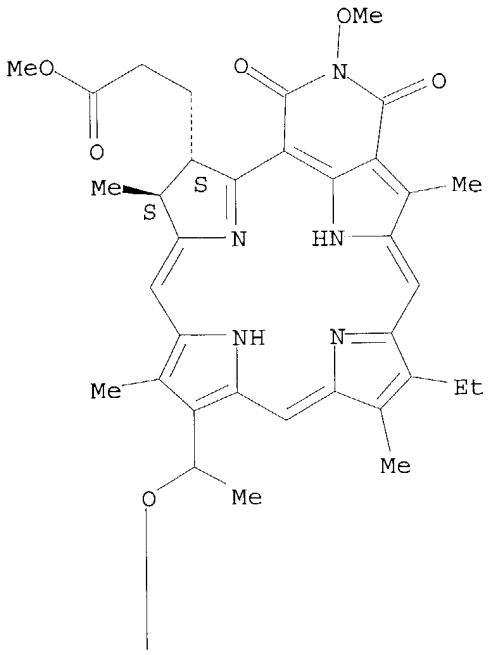
PAGE 2-A



RN 698392-35-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-4-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-19-methoxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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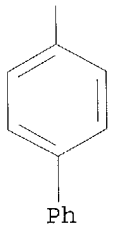
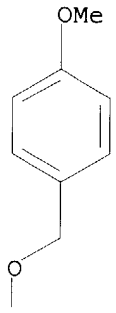


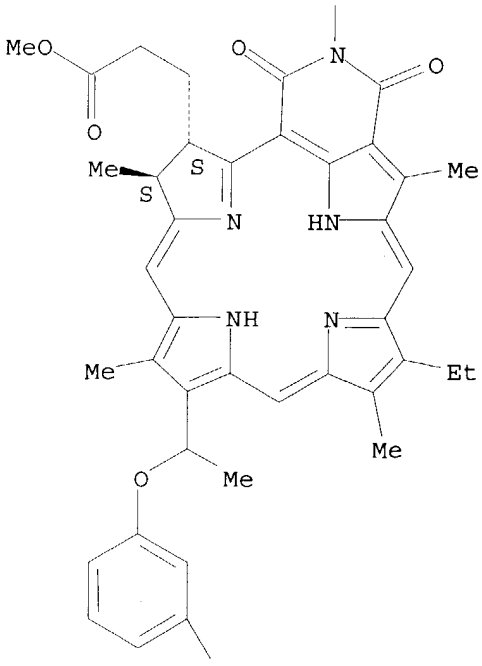
RN 698392-36-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-([1,1'-biphenyl]-3-yloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-19-[(4-methoxyphenyl)methoxy]-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



L18 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:100491 HCAPLUS
DOCUMENT NUMBER: 140:159741
TITLE: Method for using chlorin and bacteriochlorin-based aminophenyl DTPA and N2S2 conjugates for MR contrast media and radiopharmaceuticals
INVENTOR(S): Pandey, Ravindra K.; Grossman, Zachary; Kanter, Peter; Dougherty, Thomas J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 25 pp., Cont.-in-part of U.S. Ser. No. 739,155.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004022737	A1	20040205	US 2003-390438	20030317
US 2001046983	A1	20011129	US 2000-739155	20001218
US 6534040	B2	20030318		
AT 264862	E	20040515	AT 2000-128019	20001220
JP 2001335578	A2	20011204	JP 2000-404615	20001225
PRIORITY APPLN. INFO.:			US 1999-171961P	P 19991223
			US 2000-739155	A2 20001218

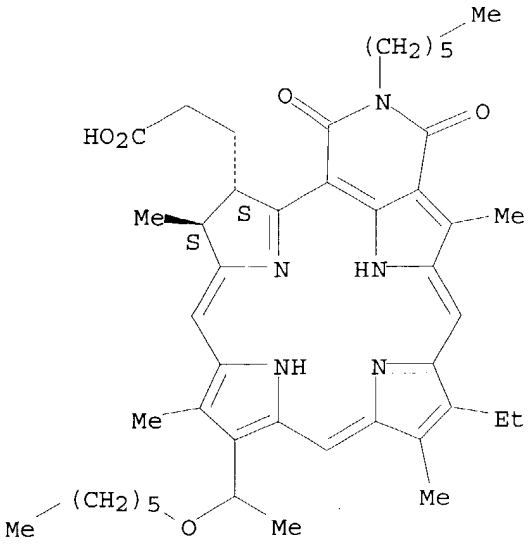
OTHER SOURCE(S): MARPAT 140:159741

AB A method for MR imaging that comprises conducting the MR imaging after injecting compns. that are chemical combination of porphyrins, chlorins, bacteriochlorins, and related tetra-pyrrolic compds. with radioactive elements such as technetium 99, gadolinium, indium 111 and radioactive iodine. When the element can form cations, the compound is usually a chelate with the porphyrin or chlorin structure. When the element forms anions, the compound is usually a direct chemical combination of the radioactive element into the porphyrin or chlorin structure. The method uses the compds. of the invention for diagnostic imaging of hyperproliferative tissue such as tumors and new blood vessel growth as is associated with the wet form of age related macular degeneration.

IT **346432-58-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chlorin- and bacteriochlorin-based aminophenyl DTPA and N2S2 conjugates for MR contrast media and radiopharmaceuticals)

RN 346432-58-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:20489 HCAPLUS
DOCUMENT NUMBER: 140:73251
TITLE: Fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy
INVENTOR(S): Pandey, Ravindra K.; Potter, William R.; Dougherty, Thomas J.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002476	A2	20040108	WO 2003-US20427	20030627
WO 2004002476	C2	20040401		
WO 2004002476	A3	20040513		
WO 2004002476	B1	20040708		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2004044197	A1	20040304	US 2003-607922	20030627

PRIORITY APPLN. INFO.: US 2002-392473P P 20020627
OTHER SOURCE(S): MARPAT 140:73251
AB Provided herein are compds. for detection, diagnosis and treatment of target tissues or target compns., including hyperproliferative tissues

such as tumors, using photodynamic methods. In particular, photosensitizer compds. that collect in hyperproliferative tissue are provided. In another embodiment, compds. that absorb light at a wavelength of from about 700 to about 850 nm are provided. In a further embodiment, compds. that are detectable by magnetic resonance imaging are provided. Among examples provided are preparation of purpurinimides and their potential photodynamic efficacy against tumor cells, against Helicobacter pylori, against pulmonary tuberculosis, and against otitis media.

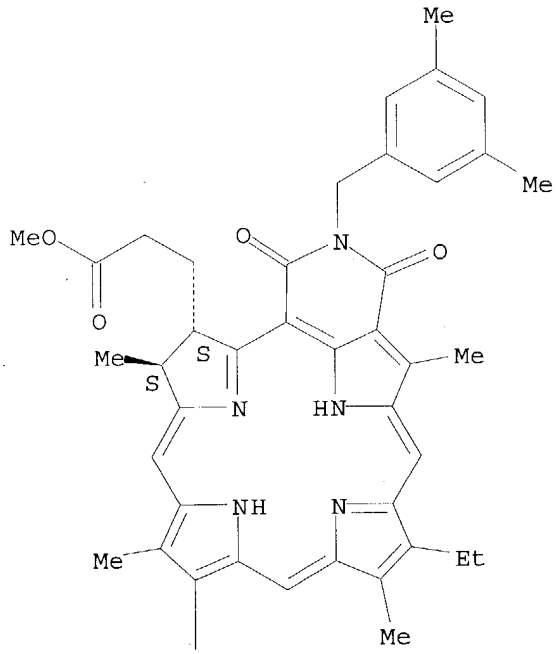
IT **503273-83-4P 503273-84-5P 503273-85-6P**
503273-86-7P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy)

RN 503273-83-4 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-(1-butoxyethyl)-19-[(3,5-dimethylphenyl)methyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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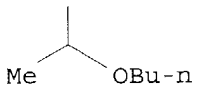
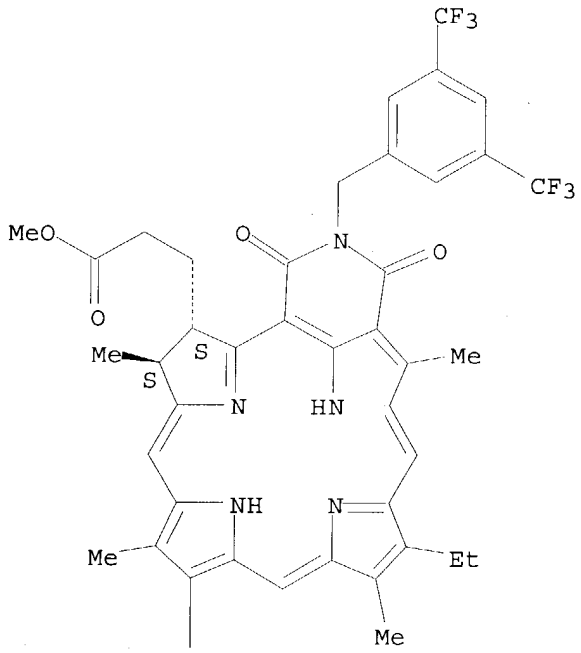


RN 503273-84-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-(1-butoxyethyl)-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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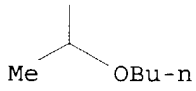
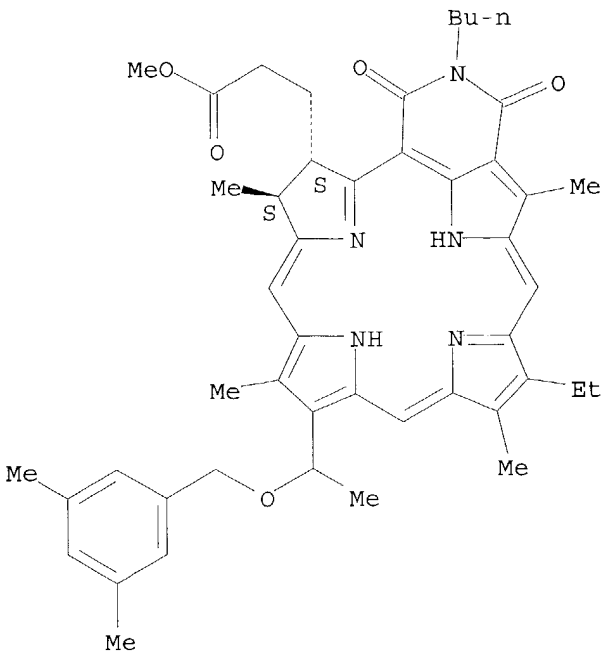


RN 503273-85-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-butyl-10-[1-[(3,5-dimethylphenyl)methoxy]ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

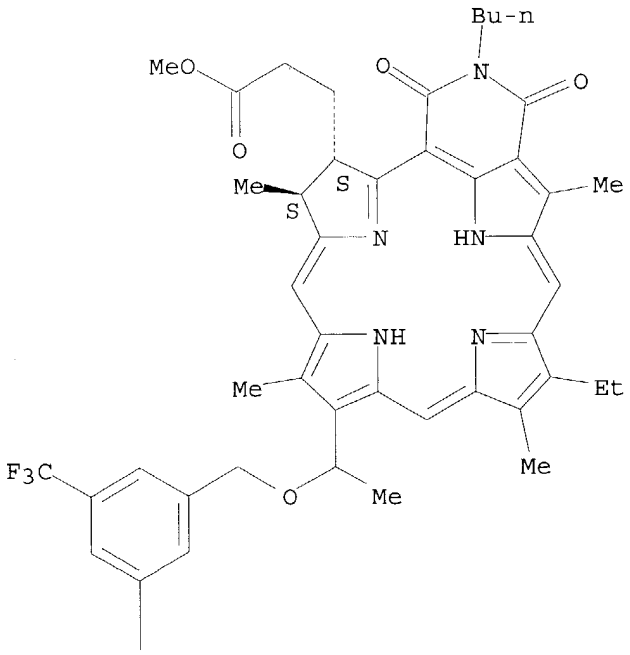
Absolute stereochemistry.



RN 503273-86-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-[[3,5-bis(trifluoromethyl)phenyl]methoxy]ethyl]-19-butyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

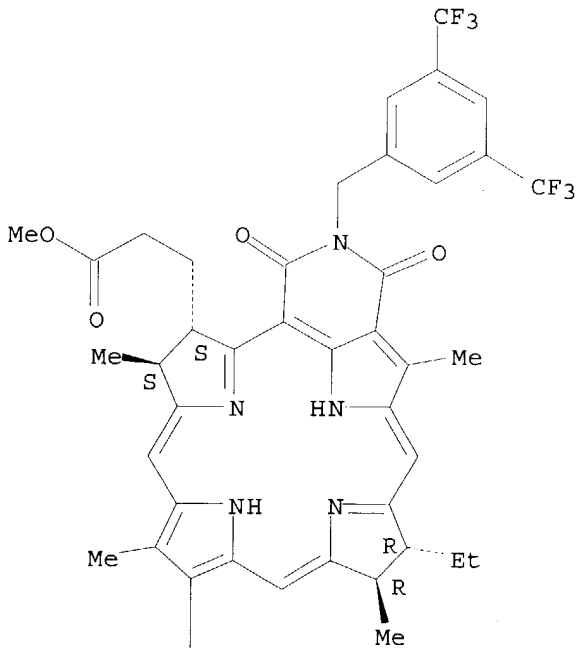
IT **639857-53-7P 639857-55-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy)

RN 639857-53-7 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-10-[1-(heptyloxy)ethyl]-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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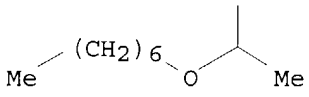
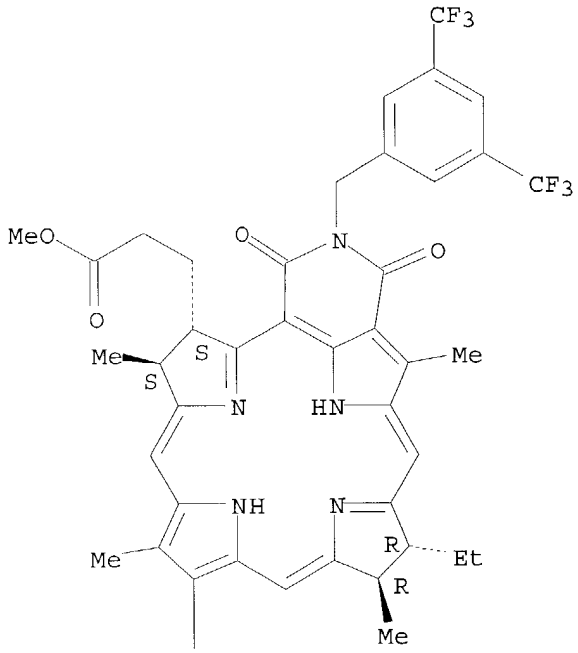


RN 639857-55-9 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-[1-[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]ethyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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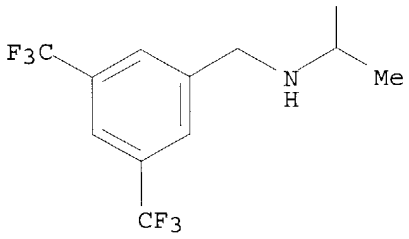
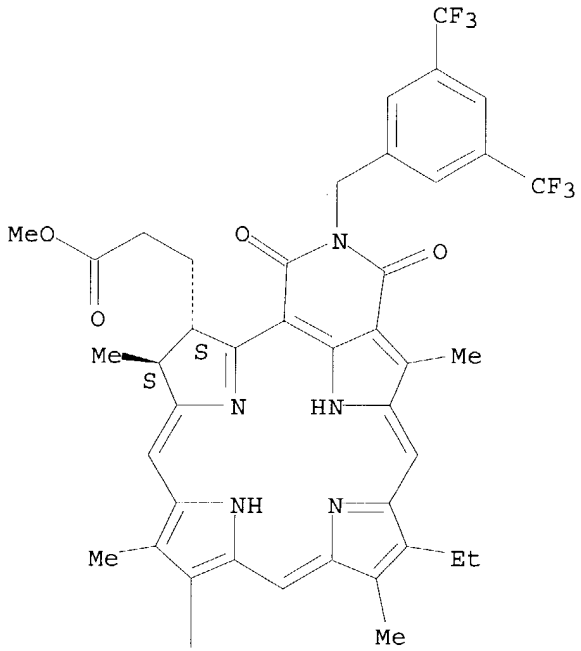


IT **639857-48-0P 639857-49-1P 639857-50-4P**
639857-51-5P 639857-52-6P 639857-54-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy)
RN 639857-48-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-

b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,15,16,18,19,20-hexahydro-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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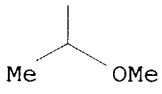
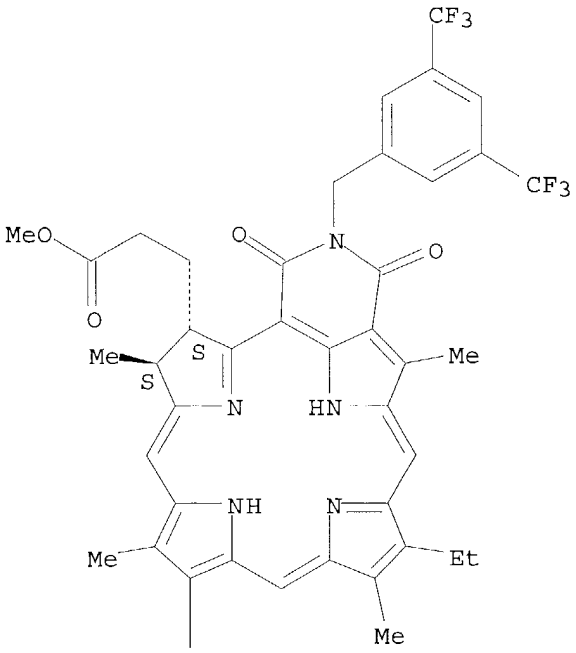


RN 639857-49-1 HCAPLUS

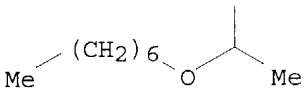
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-10-[1-(heptyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



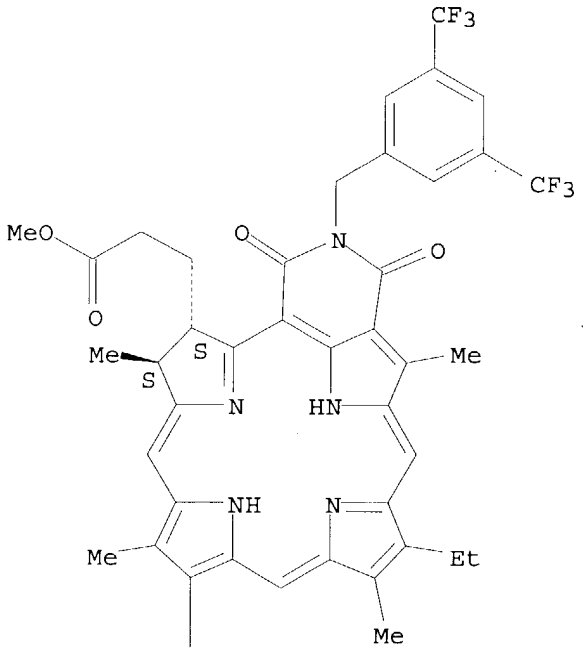
PAGE 2-A



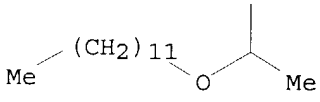
RN 639857-50-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-[1-(dodecyloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



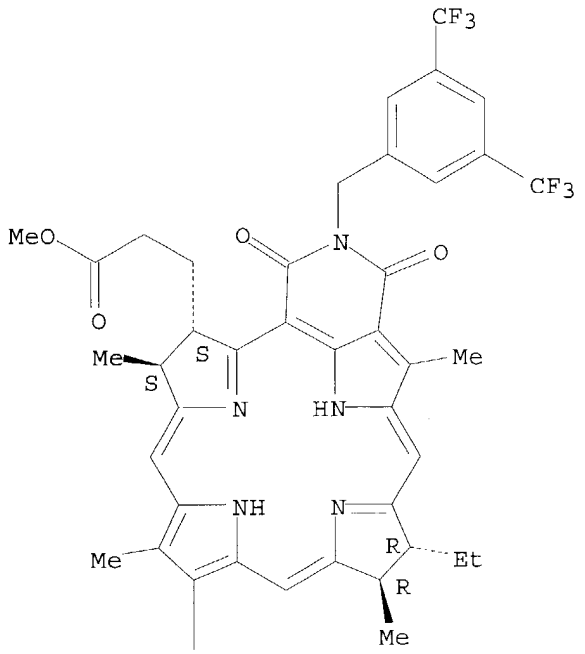
PAGE 2-A



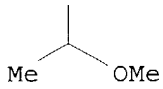
RN 639857-51-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



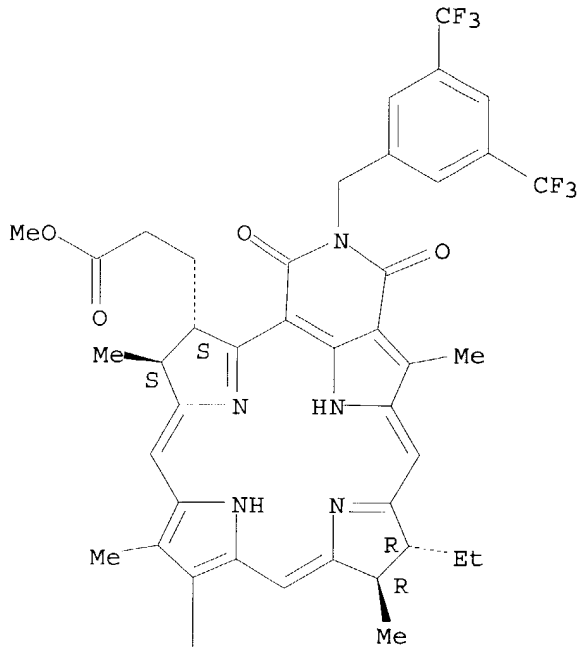
PAGE 2-A



RN 639857-52-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-(1-butoxyethyl)-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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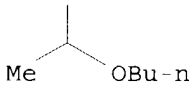
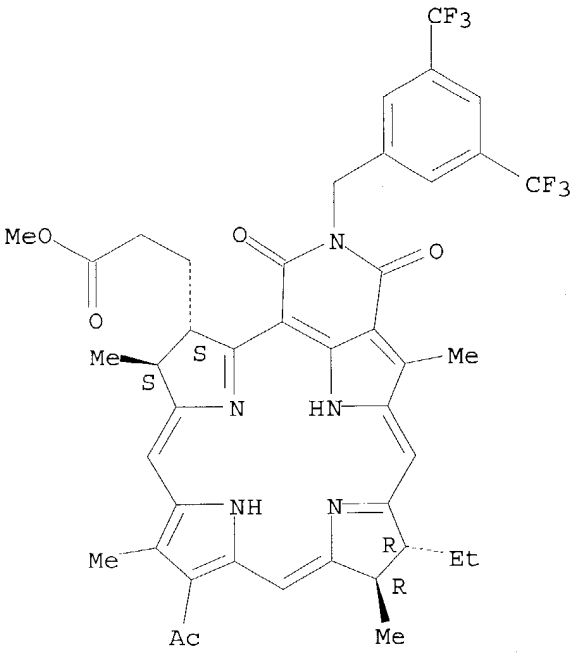


RN 639857-54-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



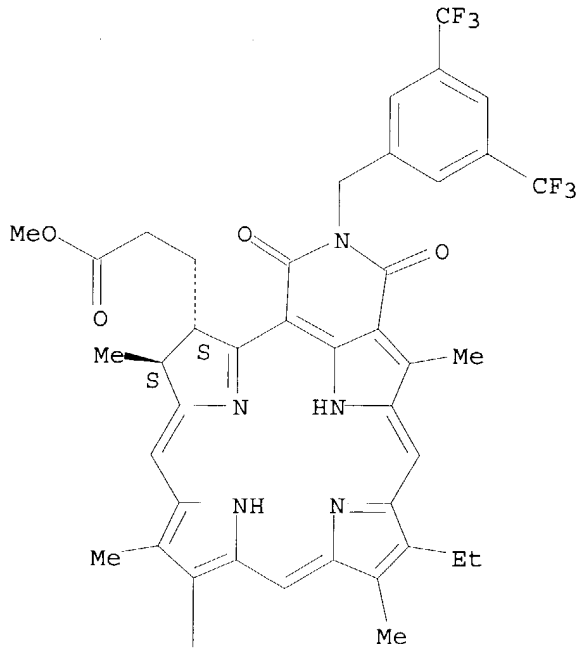
IT **503273-82-3 639857-56-0 639857-57-1**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fluorinated photosensitizers related to chlorins and bacteriochlorins for photodynamic therapy)

RN 503273-82-3 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-ethenyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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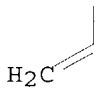
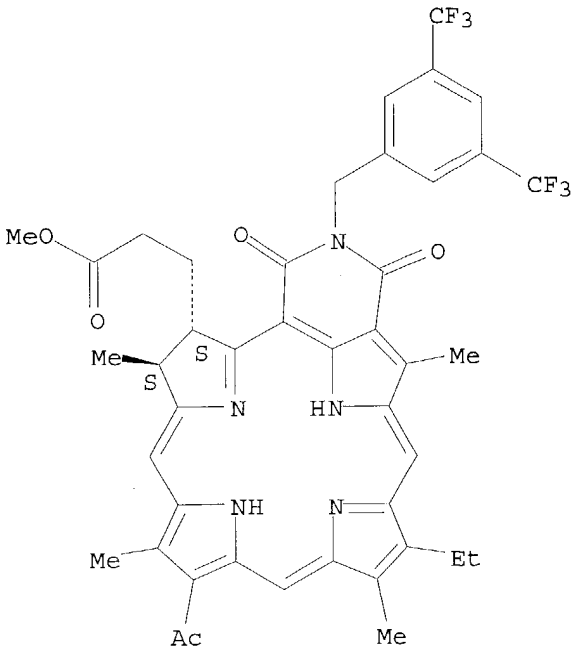


RN 639857-56-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

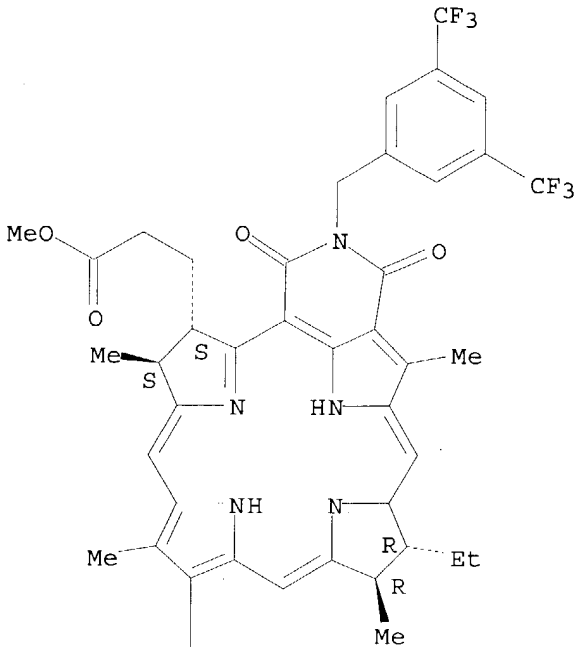
Absolute stereochemistry.



RN 639857-57-1 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-[1-[[[3,5-bis(trifluoromethyl)phenyl]methyl]imino]ethyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



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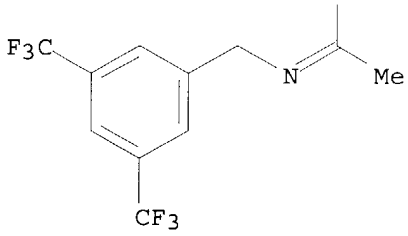


L18 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:860622 HCAPLUS

DOCUMENT NUMBER: 140:76936

TITLE: Synthesis, Comparative Photosensitizing Efficacy, Human Serum Albumin (Site II) Binding Ability, and Intracellular Localization Characteristics of Novel Benzobacteriochlorins Derived from vic-Dihydroxybacteriochlorins

AUTHOR(S): Li, Guolin; Graham, Andrew; Chen, Yihui; Dobhal, Mahabeer P.; Morgan, Janet; Zheng, Gang; Kozyrev, Andrei; Oseroff, Allan; Dougherty, Thomas J.; Pandey, Ravindra K.

CORPORATE SOURCE: Photodynamic Therapy Center, Department of Dermatology, Department of Nuclear Medicine and Radiology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA

SOURCE: Journal of Medicinal Chemistry (2003), 46(25),

5349-5359
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:76936

AB In a sequence of reactions, Me mesopyropheophorbide a, mesochlorin e6 tri-Me ester, mesochlorin p6 tri-Me ester, mesopurpurin-18-N-hexylimide Me ester, and mesopurpurin-18-N-3,5-bis(trifluoromethyl)benzylimide Me ester were synthesized from chlorophyll-a. These chlorins on reacting with osmium tetraoxide produced the corresponding vic-dihydroxybacteriochlorins. The 8-vinylchlorins obtained by refluxing the related vic-dihydroxybacteriochlorins in o-dichlorobenzene were individually treated with di-Me acetylenedicarboxylate (DMAD) under Diels-Alder reaction conditions. The intermediate adducts on 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) treatment rearranged to the corresponding stable benzobacteriochlorins, exhibiting the longest wavelength absorption in the range of 737 to 805 nm. In preliminary in vitro (RIF tumor cells) and in vivo screening (C3H/HeJ mice bearing RIF tumors), some of these compds. were found to be quite effective. Under similar treatment conditions (drug dose: 5.0 μmol/kg; light dose: 135 J/cm2, tumors were exposed to light for 30 min at 24 h postinjection), the benzobacteriochlorins containing N-substituted-imide ring system produced enhanced photosensitizing efficacy with limited skin phototoxicity. These compds. were also found to bind to site II of human serum albumin (HSA). However, no correlation between the binding constant values and photosensitizing efficacy was observed A competitive intracellular localization study of these novel structures with Rhodamine-123 (a mitochondrial probe) indicated their preferential localization in mitochondria, without producing any specific displacement of 3H-PK11195 (PBR probe, 3H-labeled 1-(2-chlorophenyl)-N-methyl-N-(1-methylpropyl)-3-isoquinoline carboxamide). These results suggest that the mitochondrial peripheral benzodiazepine receptor (PBR) is not the cellular binding site for this class of compds.

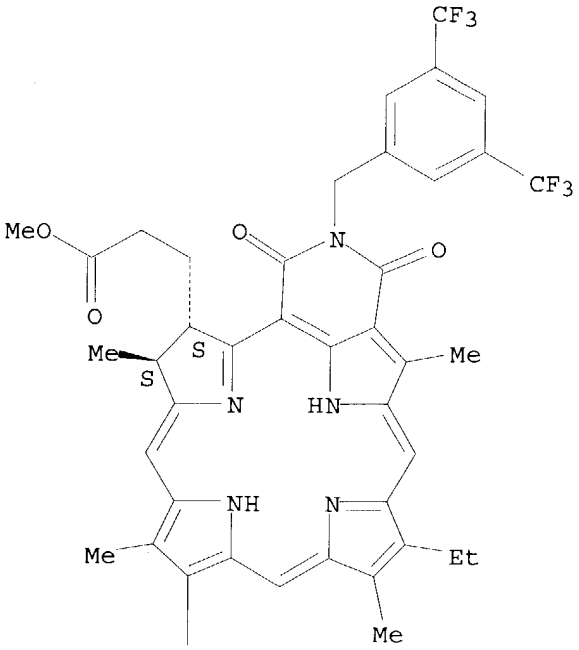
IT **503273-82-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzobacteriochlorins, their photosensitizing efficacy on RIF tumors, skin phototoxicity, human serum albumin binding, intracellular localization, and peripheral benzodiazepine receptor binding)

RN 503273-82-3 HCAPLUS

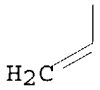
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-ethenyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

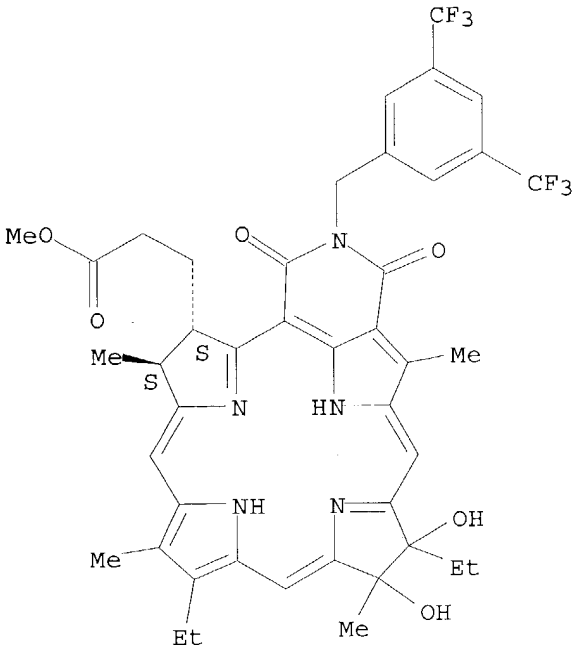


IT **538367-90-7P 538367-96-3P 639855-79-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzobacteriochlorins, their photosensitizing efficacy on RIF tumors, skin phototoxicity, human serum albumin binding, intracellular localization, and peripheral benzodiazepine receptor binding)

RN 538367-90-7 HCAPLUS

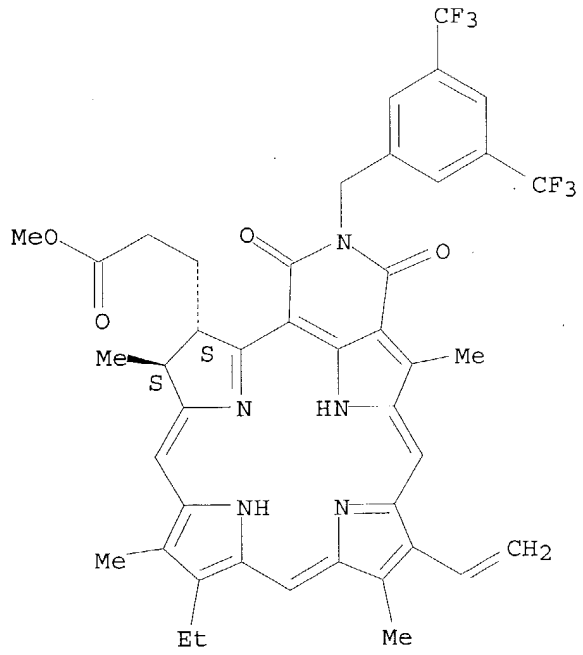
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5,10-diethyl-1,5,6,15,16,18,19,20-octahydro-5,6-dihydroxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



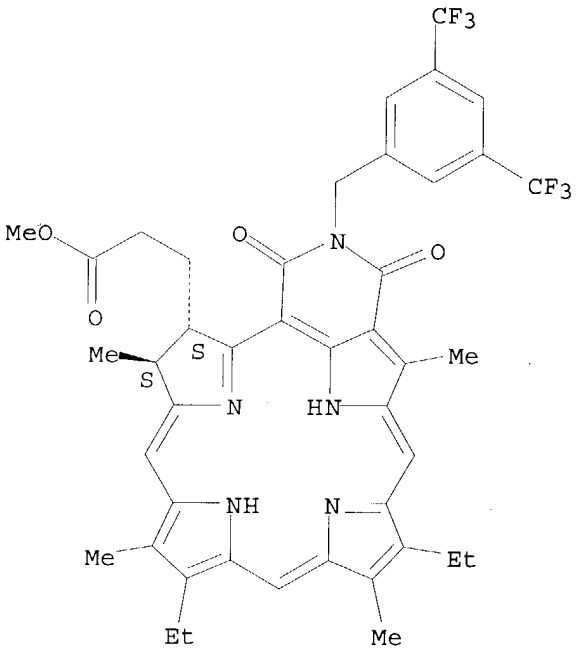
RN 538367-96-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethenyl-10-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 639855-79-1 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5,10-diethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:683489 HCAPLUS
DOCUMENT NUMBER: 140:50149
TITLE: Intramolecular electron transfer in bacteriochlorin-C60 and zinc chlorin-C60 dyads
AUTHOR(S): Ohkubo, Kei; Imahori, Hiroshi; Shao, Jianguo; Ou, Zhongping; Kadish, Karl M.; Chen, Yihui; Zheng, Gang; Pandey, Ravindra K.; Fujitsuka, Mamoru; Ito, Osamu; Fukuzumi, Shunichi
CORPORATE SOURCE: Department of Material and Life Science, Graduate School of Engineering, CREST, Japan Science and Technology Corporation, Osaka University, Osaka, 565-0871, Japan
SOURCE: Proceedings - Electrochemical Society (2002), 2002-12(Fullerenes--Volume 12: The Exciting World of Nanocages and Nanotubes), 70-81
CODEN: PESODO; ISSN: 0161-6374
PUBLISHER: Electrochemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

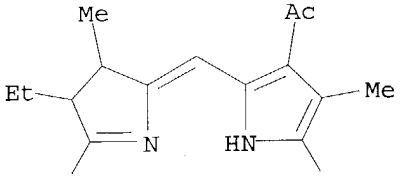
AB Rate consts. for charge separation (CS) processes in free base bacteriochlorin- and zinc chlorin-C60 dyads were determined by fluorescence lifetime measurements of the dyads. The charge recombination (CR) rate consts. of the dyads were determined using laser flash photolysis. Photoexcitation of the zinc chlorin-C60 dyad results in formation of long-lived radical ion pair which has absorption maxima at 790 and 1000 nm due to the zinc chlorin radical cation and the C60 radical anion, resp. Photoexcitation of the free-base bacteriochlorin-C60 dyad with the same short linkage leads to formation of the radical ion pair which decays quickly to the triplet excited state of the bacteriochlorin moiety. The driving force dependence of the electron transfer rate consts. of the dyads with a short spacer affords a small reorganization energy (λ) compared with the λ value of zinc porphyrin-C60 dyads with longer spacers.

IT **478978-75-5**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(dyad; photochem. and electrochem. study of free base bacteriochlorin-C60 and zinc chlorin-C60 dyads)

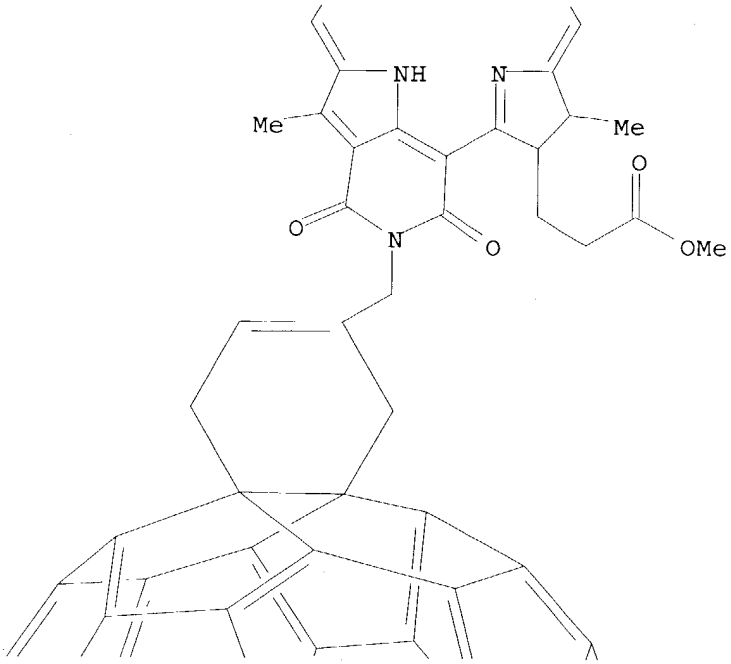
RN 478978-75-5 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[(3',6'-dihydrobenzo[1,9][5,6]fulleren-C60-Ih-4'-yl)methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15-trimethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

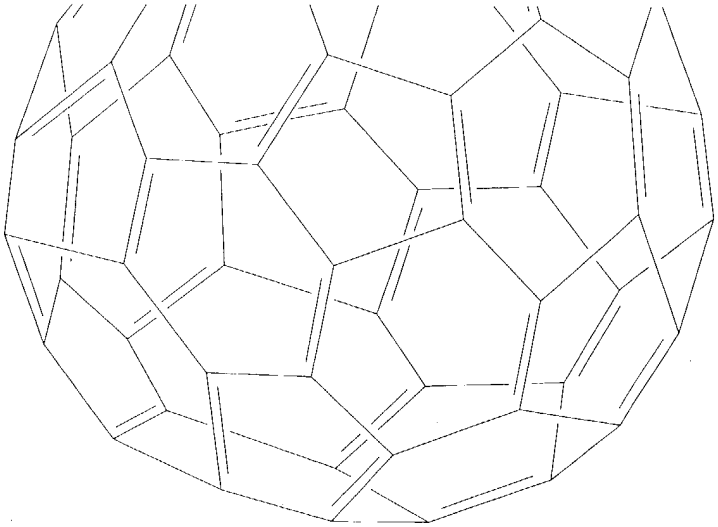
PAGE 1-A



PAGE 2-A



PAGE 3-A



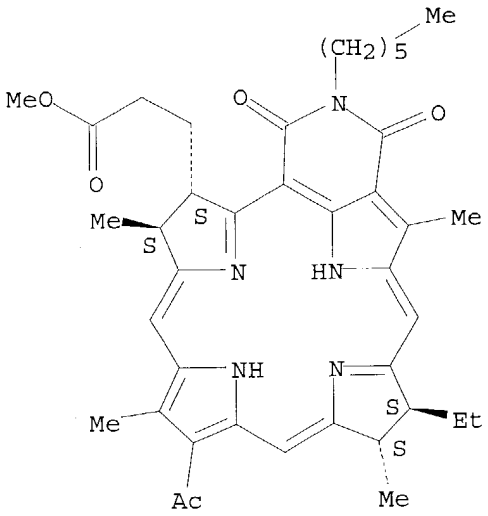
IT **438627-03-3**
RL: PRP (Properties)
(reference compound; photochem. and electrochem. study of free base bacteriochlorin-C60 and zinc chlorin-C60 dyads)

RN 438627-03-3 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-1,5,6,15,16,18,19,20-

octahydro-5-ethyl-19-hexyl-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:284656 HCAPLUS
DOCUMENT NUMBER: 139:22042
TITLE: Thermolysis of vic-Dihydroxybacteriochlorins: Effect of the Nature of Substrates in Directing the Formation of Chlorin-Chlorin Dimers with Fixed and Flexible Orientations and Their Preliminary in Vitro Photosensitizing Efficacy
AUTHOR(S): Li, Guolin; Dobhal, Mahabeer P.; Graham, Andrew; Shibata, Masayuki; Zheng, Gang; Kozyrev, Andrei; Pandey, Ravindra K.
CORPORATE SOURCE: Chemistry Division, Photodynamic Therapy Center, Department of Nuclear Medicine and Radiology and Department of Dermatology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Journal of Organic Chemistry (2003), 68(10), 3762-3772
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:22042

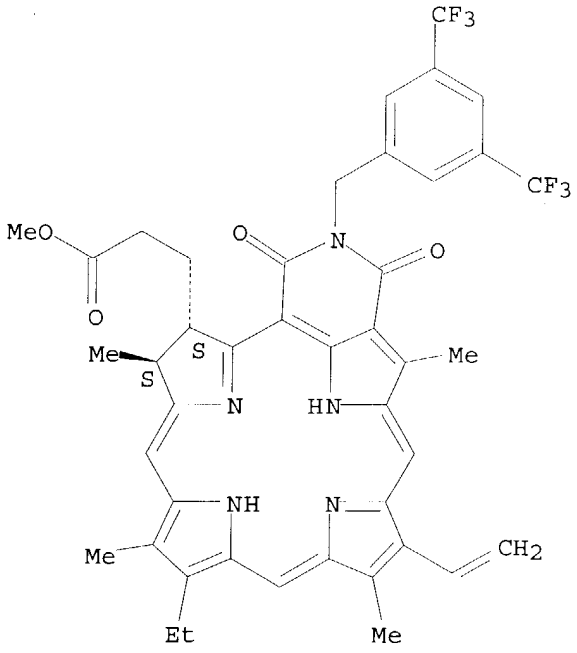
AB The thermolysis products obtained by refluxing a series of vic-dihydroxychlorins in o-dichlorobenzene are characterized. Depending on the nature of substrates, this methodol. provides an access for novel carbon-carbon linked chlorin-chlorin dimers and chlorin-porphyrin dimers with fixed and flexible orientations. The configuration of the linkers in the sym. and unsym. dimers was confirmed by extensive NMR (COSY, ROESY) and mol. modeling studies. The mol. modeling studies of the energy-optimized dimers with flexible orientation confirmed that one of the chlorin units of the dimeric structure is tilted toward the opposite ring as evident by the shielding effect in the resonances of some of the

protons in the 1H NMR spectroscopy. Among the dimers with fixed orientation, compared to the free-base analogs, the related mono- and di-Zn(II) complexes produced a decreased fluorescence intensity, suggesting a possibility of the faster energy transfer via intersystem crossing (ISC) in the metalated derivs. than the corresponding free-base analogs to produce the corresponding excited triplet states. The photosensitizing efficacy of the monomers and the related dimers was also compared in radiation-induced fibrosarcoma (RIF) tumor cells at variable drug/light doses. In preliminary screening, compared to monomers, the corresponding carbon-carbon linked dimers produced enhanced photosensitizing efficacy.

IT **538367-96-3P 538367-98-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and photosensitizing efficacy of vic-dihydroxybacteriochlorin thermolysis products)

RN 538367-96-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-ethenyl-10-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

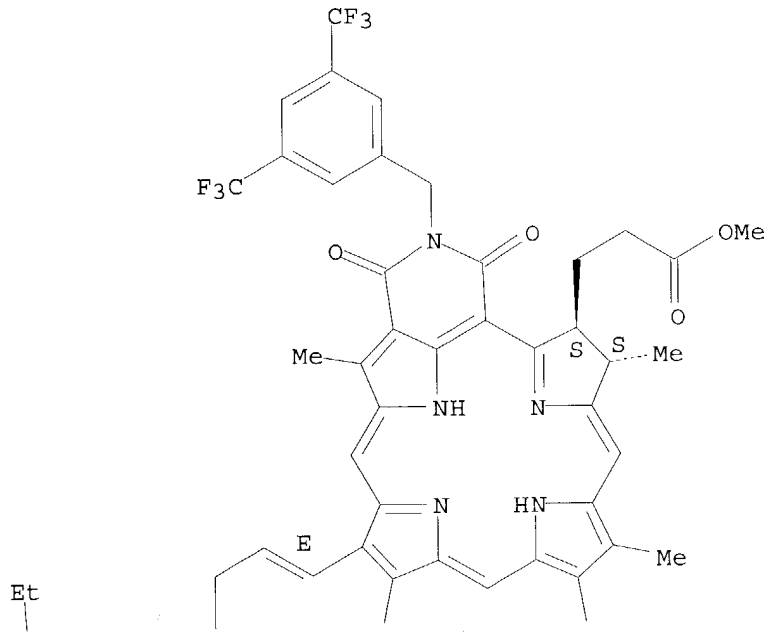


RN 538367-98-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5-[(1E)-3-[(15S,16S)-19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5,10-diethyl-1,15,16,18,19,20-hexahydro-16-(3-methoxy-3-oxopropyl)-11,15,22-trimethyl-18,20-dioxo-9,12-imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecin-6-yl]-1-

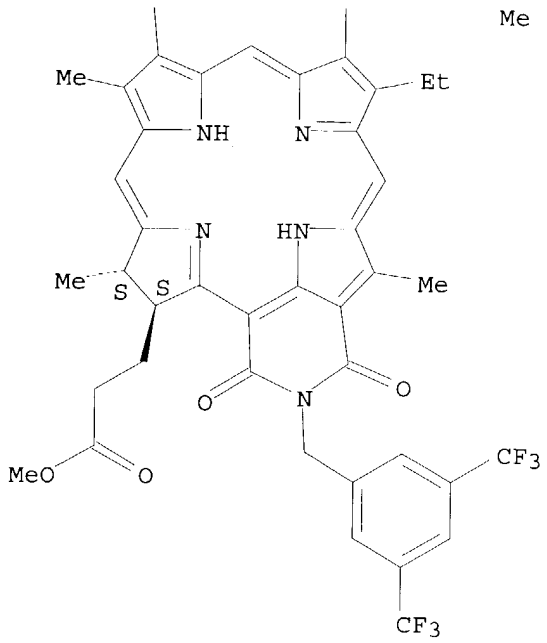
propenyl]-10-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

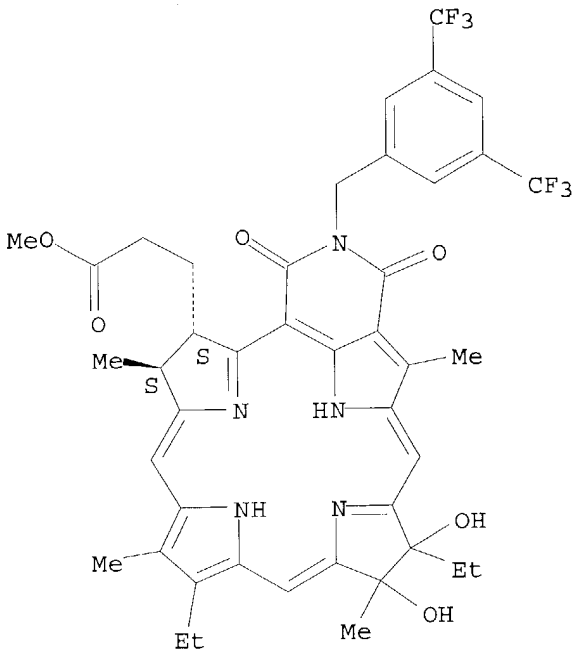


PAGE 2-A



IT **538367-90-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and photosensitizing efficacy of vic-dihydroxybacteriochlorin thermolysis products)
RN 538367-90-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-5,10-diethyl-1,5,6,15,16,18,19,20-octahydro-5,6-dihydroxy-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

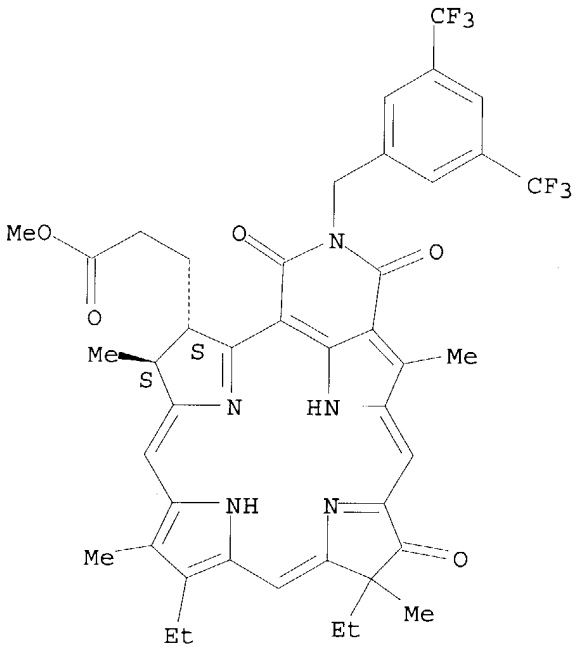


IT **538367-97-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and photosensitizing efficacy of vic-dihydroxybacteriochlorin thermolysis products)

RN 538367-97-4 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-6,10-diethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-5,18,20-trioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:282317 HCAPLUS
DOCUMENT NUMBER: 138:304082
TITLE: Preparation of photosensitizing carbamate derivatives useful in photodynamic therapy
INVENTOR(S): Robinson, Byron C.; Phadke, Avinash
PATENT ASSIGNEE(S): Miravant Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003028628	A2	20030410	WO 2002-US29832	20021002
WO 2003028628	A3	20040108		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1450790	A2	20040901	EP 2002-773496	20021002
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
PRIORITY APPLN. INFO.: US 2001-326427P P 20011003
WO 2002-US29832 W 20021002

OTHER SOURCE(S): MARPAT 138:304082

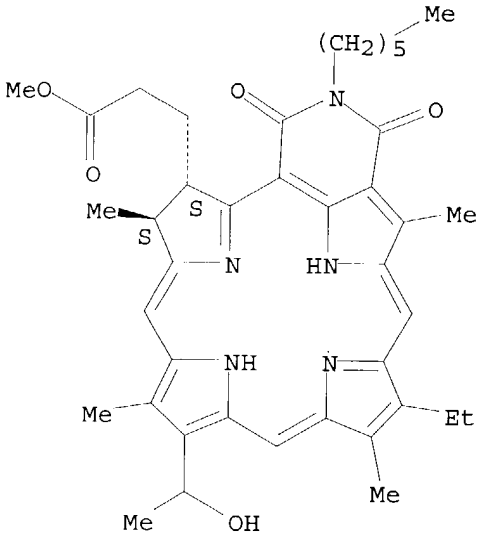
AB Carbamate compds., e.g., I [R1 - R14 = H, halogen, (un)substituted C1-20-alkyl, heteroalkyl, haloalkyl, heterohaloalkyl, cycloalkyl, (un)substituted aryl, (un)substituted alkenyl, (un)substituted alkynyl, amide ester, ether, polyether, alkoxy, arylaoxy, haloalkoxy, NH2, alkylcarbonyloxy, alkoxycarbonyl, aryloxybarbonyl, azo, arylcarbonyloxy, alkoxycarbonyloxy, aryloxycarbonyloxy, sulfinyl, sulfonyl, silyl, carbamoyl, heterocyclyl, NO2, NO, OCHO, isocyano, cyanate, isocyanate, thiocyanate isothiocyanate, N(alkyl)2, N(aryl)2, CH:CH-aryl, CH:CHCH2NMe2, CH:CHCH2N+Me3A-,CH:N+(alkyl)2A-, N+(alkyl)3A-, CN, OH, CHO, Ac, CO-alkyl, CO2H, CO2Na, CO2K, etc.; R3R4 = bond; R12R13 = bond; R7R8 = :O; R9R10 = :O; A = physiol. acceptable counter ion; M = 2H, metal cation, photoactive metal ion (e.g., Ga+3, Pt2+, Pd2+, Sn4+, In+3, Ge4+, Si4+, Al3+, Zn2+, Mg2+)], their pharmaceutically acceptable salts, prodrugs, solvates or metabolites, and compns. useful in photodynamic therapy for treating ophthalmic, cardiovascular, and skin diseases are described. Thus, porphyrin carbamate II was prepared from 2-desvinyl-2-(hydroxymethyl)pyropheophorbide a Me ester via reaction with carbonyl diimidazole in CH2Cl2 containing DMAP followed my amidation with HN:C(NMe2)2. Antitumor activity of II was determined (@ 1.0 μM/Kg it took 23 days for regrowth after PDT); its effect on exptl.-induced corneal neovascularization was determined (@ 1.0 μM/Kg 0.51-1.0 mm closure at 28 days after PDT); its effect on normal choriocapillaris as model for neovasculature was tested (@ 1.5 μM/Kg 51-75% closure at 28 days after PDT); its effect on exptl.-induced choroidal neovascularization (CNV) was determined (@ 3.0 μM/Kg closure of CNV at 10 - 40 min. intervals at 28 days after PDT).

IT **507485-71-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbamylation of; preparation of photosensitizing carbamate derivs. useful in photodynamic therapy)

RN 507485-71-4 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-10-(1-hydroxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

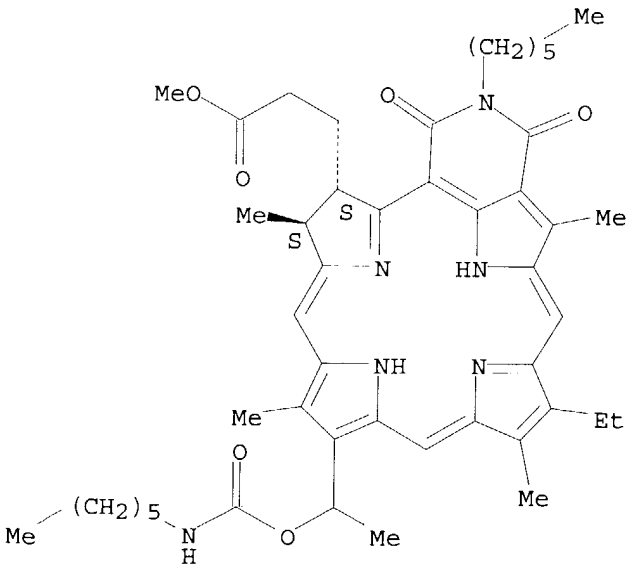


IT **507226-85-9P 507226-86-0P 507226-87-1P**
507226-90-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of photosensitizing carbamate derivs. useful in photodynamic therapy)

RN 507226-85-9 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-[[(hexylamino)carbonyl]oxy]ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

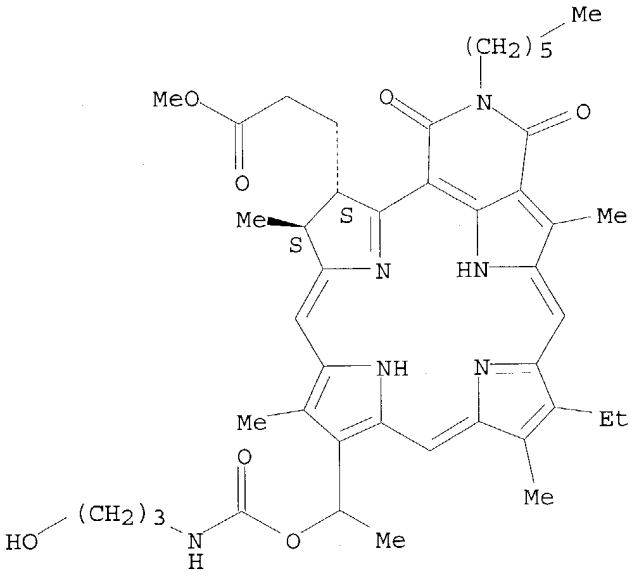
Absolute stereochemistry.



RN 507226-86-0 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-10-[1-[[[(3-hydroxypropyl)amino]carbonyl]oxy]ethyl]-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

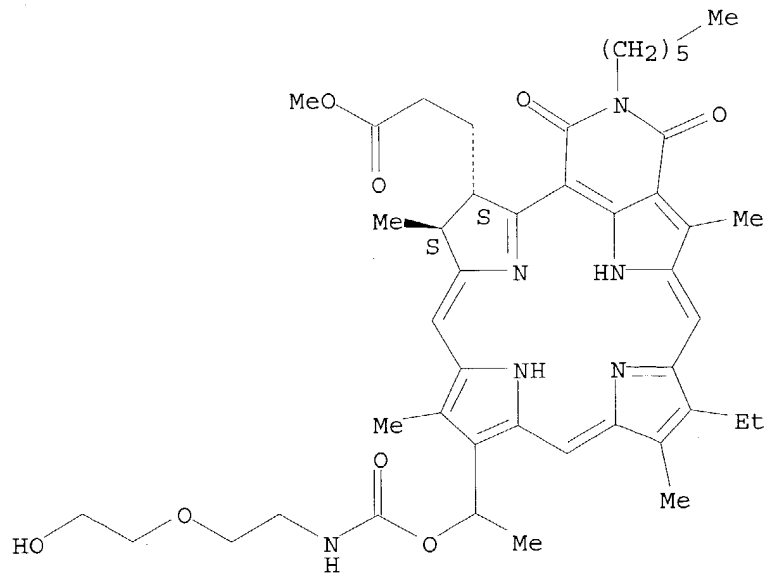
Absolute stereochemistry.



RN 507226-87-1 HCAPLUS

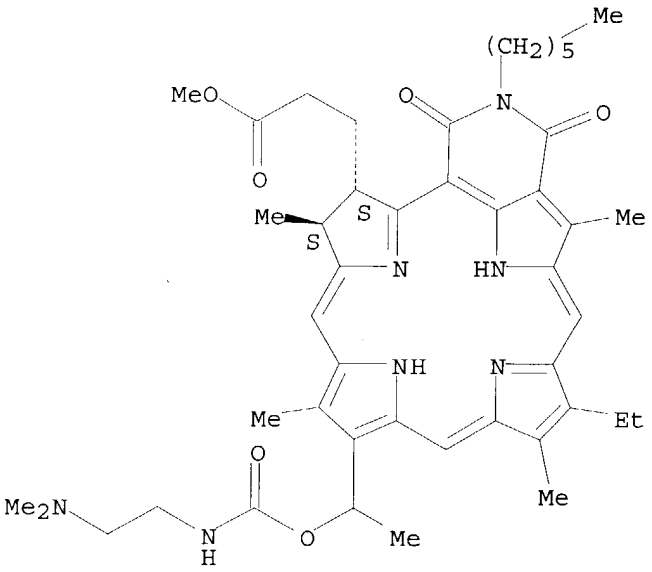
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-10-[1-[[[[2-(2-hydroxyethoxy)ethyl]amino]carbonyl]oxy]ethyl]-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 507226-90-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-[[[[2-(dimethylamino)ethyl]amino]carbonyl]oxy]ethyl]-5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:222134 HCAPLUS
DOCUMENT NUMBER: 138:264768
TITLE: Preparation of chlorin and bacteriochlorin-based difunctional aminophenyl DTPA and N2S2 conjugates for MR contrast media and radiopharmaceuticals
INVENTOR(S): Pandey, Ravindra K.; Grossman, Zachary; Kanter, Peter; Dougherty, Thomas J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 31 pp., Cont.-in-part of U.S. Ser. No. 739,155.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003053949	A1	20030320	US 2002-177129	20020620
US 2001046983	A1	20011129	US 2000-739155	20001218
US 6534040	B2	20030318		
AT 264862	E	20040515	AT 2000-128019	20001220
JP 2001335578	A2	20011204	JP 2000-404615	20001225
EP 1374897	A1	20040102	EP 2003-101773	20030617
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

JP 2004026828	A2	20040129	JP 2003-177849	20030623
PRIORITY APPLN. INFO.:			US 1999-171961P	P 19991223
			US 2000-739155	A2 20001218
			US 2002-177129	A 20020620

OTHER SOURCE(S): MARPAT 138:264768

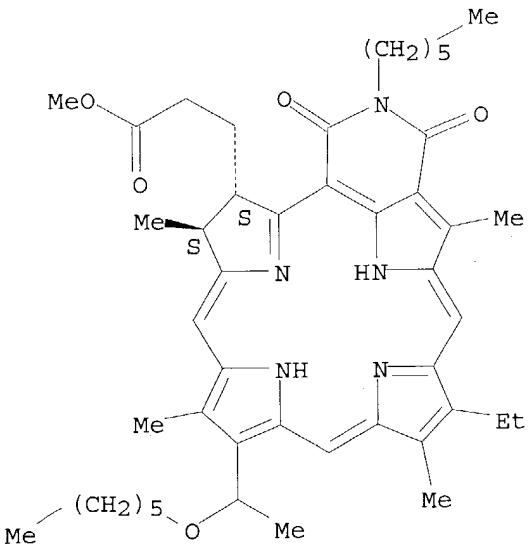
AB Compds. are prepared comprising a chemical combination of a photodynamic tetra-pyrrolic compound with a plurality of radionuclide element atoms such that the compound may be used to enhance MR imaging and also be used as a photodynamic compound for use in photodynamic therapy to treat hyperproliferative tissue. The preferred compds. have the structural formula (I) where R1, R2, R2a R3, R3a R4, R5, R5a R6, R7, R7a and R8 cumulatively contain at least two functional groups that will complex or combine with an MR imaging enhancing element or ion. The compound is intended to include such complexes and combinations and includes the use of such compds. for MR imaging and photodynamic therapy treatment of tumors and other hyperproliferative tissue. Thus, the digadolinium complex [Gd2(H4L)(H2O)2] (H10L = I) was prepared and its use as an MRI agent demonstrated.

IT **346432-55-1P 346432-58-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chlorin-/bacteriochlorin-based difunctional aminophenyl-DTPA/N2S2 conjugates for MR imaging and photodynamic therapy treatment of tumors)

RN 346432-55-1 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

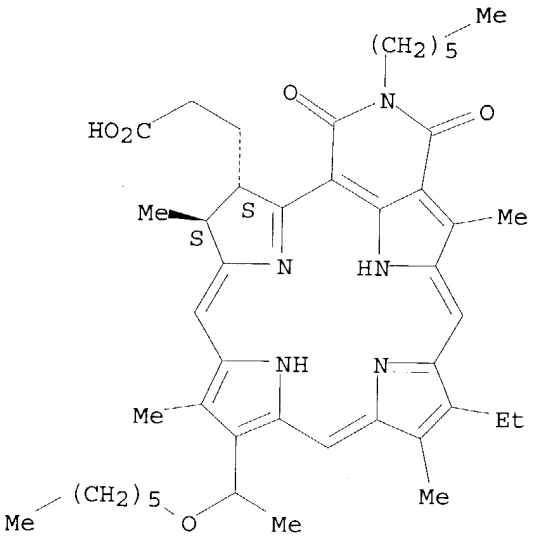
Absolute stereochemistry.



RN 346432-58-4 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:899563 HCAPLUS
DOCUMENT NUMBER: 138:267784
TITLE: A first comparative study of purpurinimide-based fluorinated vs. nonfluorinated photosensitizers for photodynamic therapy
AUTHOR(S): Gryshuk, Amy L.; Graham, Andrew; Pandey, Suresh K.; Potter, William R.; Missert, Joseph R.; Oseroff, Allan; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: Photodynamic Therapy Center, Department of Dermatology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Photochemistry and Photobiology (2002), 76(5), 555-559
CODEN: PHCBAP; ISSN: 0031-8655
PUBLISHER: American Society for Photobiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A first report on the synthesis and comparative in vitro-in vivo photosensitizing efficacy of various fluorinated and the corresponding nonfluorinated, purpurinimide-based photosensitizers is discussed. In preliminary in vivo screening, compared with the nonfluorinated analogs, purpurinimides bearing trifluoromethyl substituents showed enhanced photosensitizing efficacy. Among compds. (isomers) with similar lipophilicity, the position of the substituents was found to play a decisive role in biol. efficacy.

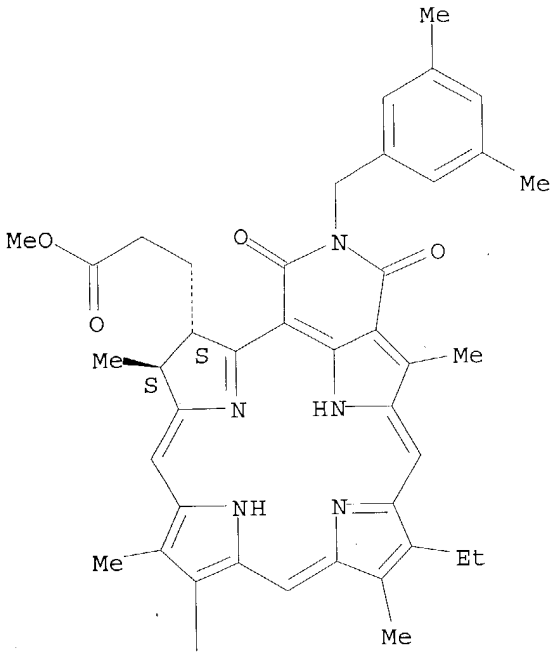
IT **503273-83-4P 503273-84-5P 503273-85-6P 503273-86-7P**
RL: DGN (Diagnostic use); PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(purpurinimide-based fluorinated vs. nonfluorinated PDT photosensitizers preparation and tumor/skin uptake)

RN 503273-83-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-(1-butoxyethyl)-19-[(3,5-

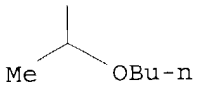
dimethylphenyl)methyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



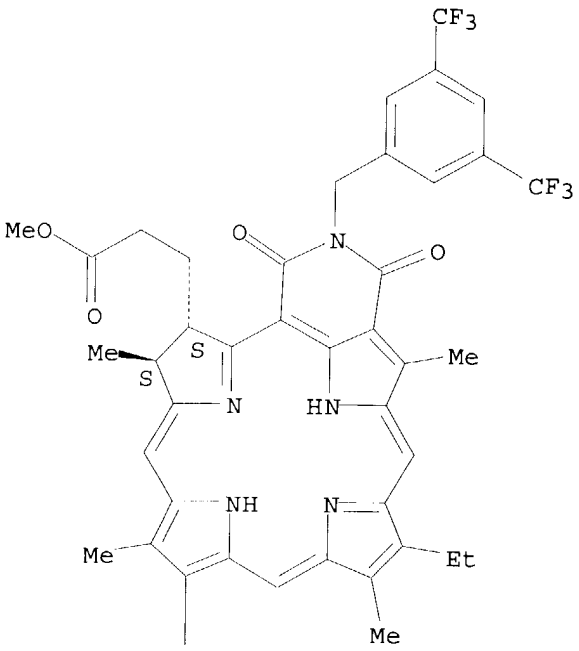
PAGE 2-A



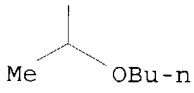
RN 503273-84-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-(1-butoxyethyl)-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

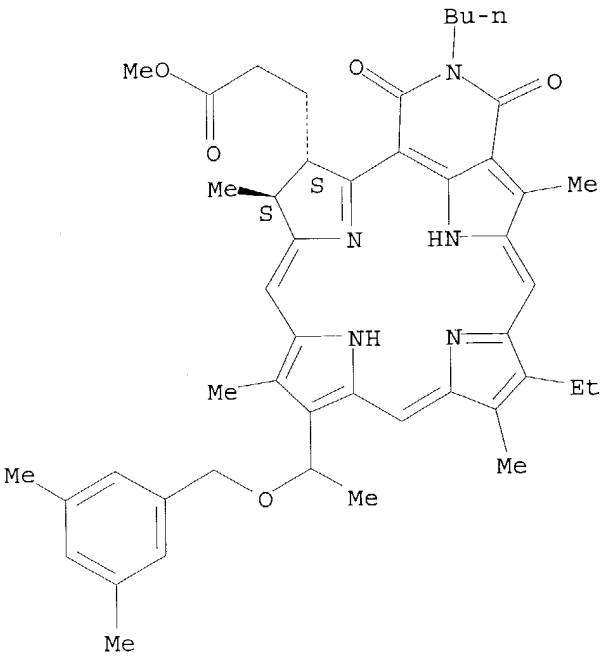


PAGE 2-A



RN 503273-85-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-butyl-10-[1-[(3,5-dimethylphenyl)methoxy]ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

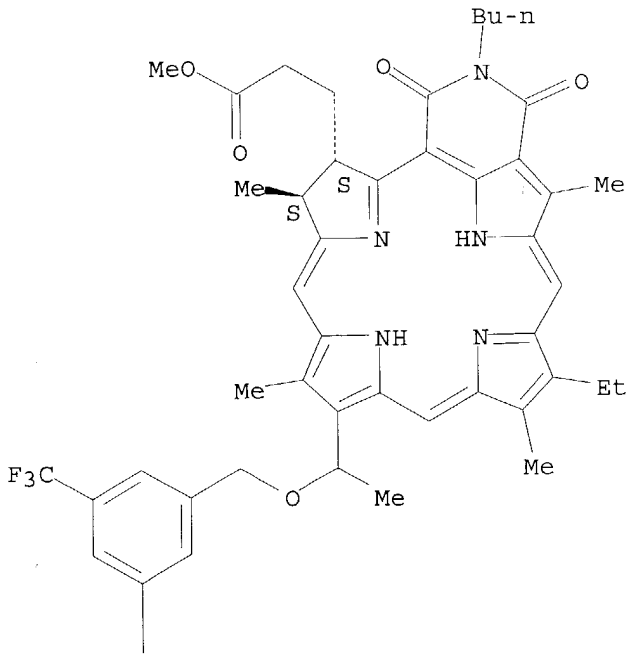
Absolute stereochemistry.



RN 503273-86-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-[[3,5-bis(trifluoromethyl)phenyl]methoxy]ethyl]-19-butyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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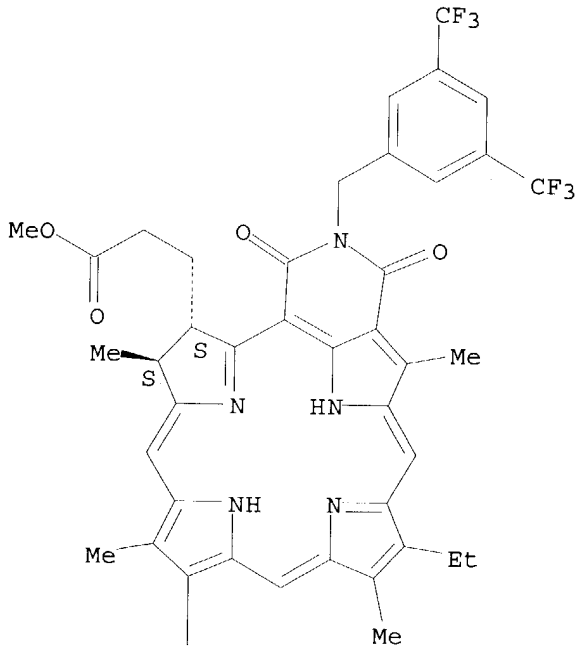
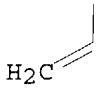
IT **503273-82-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(purpurinimide-based fluorinated vs. nonfluorinated PDT photosensitizers preparation and tumor/skin uptake)
RN 503273-82-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-[[3,5-bis(trifluoromethyl)phenyl]methyl]-10-ethenyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

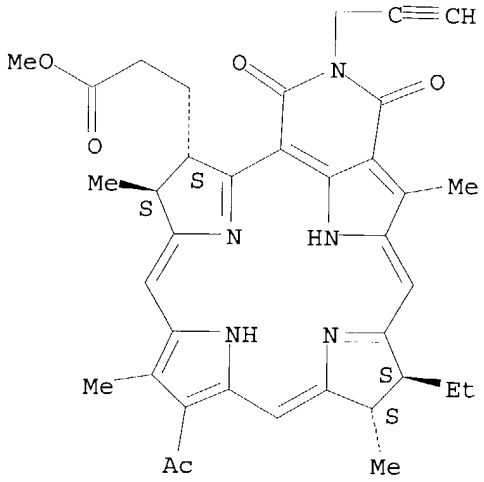
L18 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:801953 HCAPLUS
DOCUMENT NUMBER: 138:47144
TITLE: Small Reorganization Energy of Intramolecular Electron Transfer in Fullerene-Based Dyads with Short Linkage
AUTHOR(S): Ohkubo, Kei; Imahori, Hiroshi; Shao, Jianguo; Ou, Zhongping; Kadish, Karl M.; Chen, Yihui; Zheng, Gang; Pandey, Ravindra K.; Fujitsuka, Mamoru; Ito, Osamu; Fukuzumi, Shunichi
CORPORATE SOURCE: Department of Material and Life Science Graduate School of Engineering, Osaka University, Osaka, 565-0871, Japan
SOURCE: Journal of Physical Chemistry A (2002), 106(46), 10991-10998
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A bacteriochlorin-C60 dyad (H2BCh-C60) and a zinc chlorin dyad (ZnCh-C60) with the same short spacer have been synthesized. The rate consts. for the charge-separation (CS) processes in these dyads were determined by fluorescence lifetime measurements of the dyads. The charge-recombination (CR) rate consts. of the dyads were determined using laser flash photolysis. The photoexcitation of the zinc chlorin-C60 dyad results in formation of the long-lived radical ion pair, which has absorption maxima at 790 and 1000 nm due to the zinc chlorin radical cation and the C60 radical anion, resp. Photoexcitation of the free-base bacteriochlorin-C60 dyad with the same short linkage leads to formation of the radical ion pair, which decays quickly to the triplet excited state of the bacteriochlorin moiety. The driving force dependence of the electron-transfer rate consts. of these dyads with a short spacer affords a small reorganization energy (λ = 0.51 eV) as compared with the λ value (0.66 eV) of zinc porphyrin-C60 dyads with a longer spacer.

IT **478945-66-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in synthesis of bacteriochlorin fullerene dyad)

RN 478945-66-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-19-(2-propynyl)-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

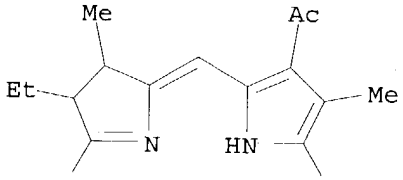


IT **478978-75-5P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(photochem. and electrochem. properties of free base bacteriochlorin- and zinc chlorin-fullerene dyads)

RN 478978-75-5 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-19-[(3',6'-dihydrobenzo[1,9][5,6]fulleren-C60-Ih-4'-yl)methyl]-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15-trimethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

PAGE 1-A



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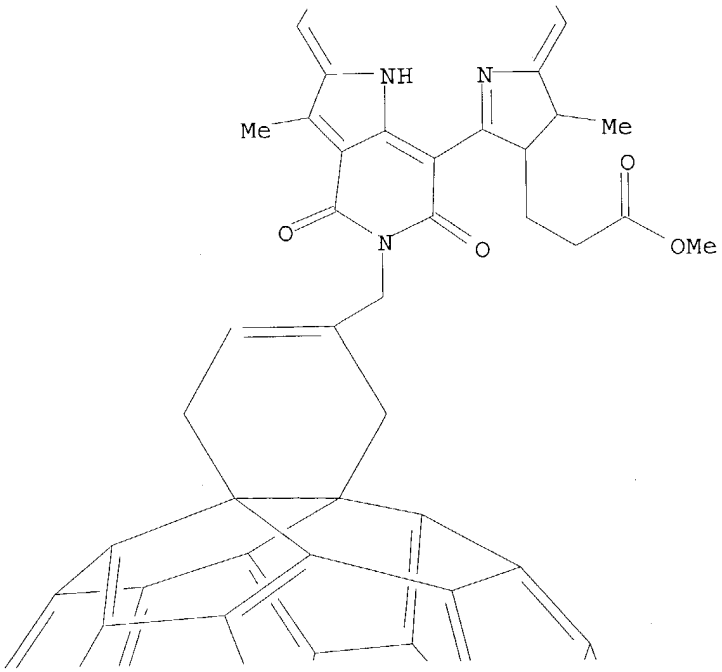

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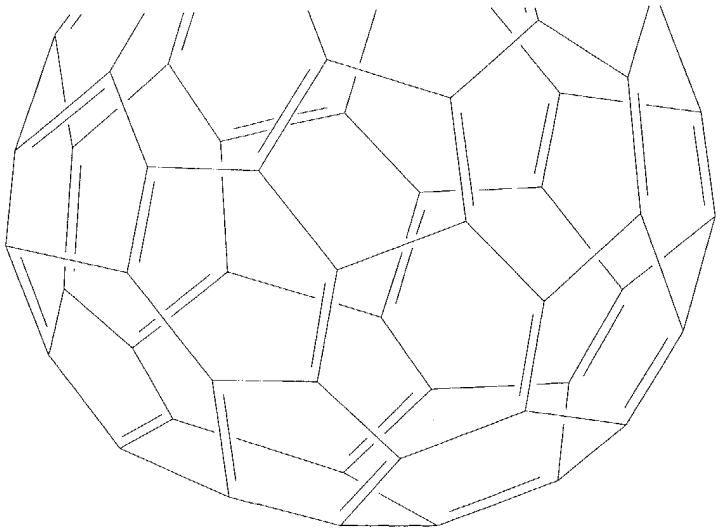
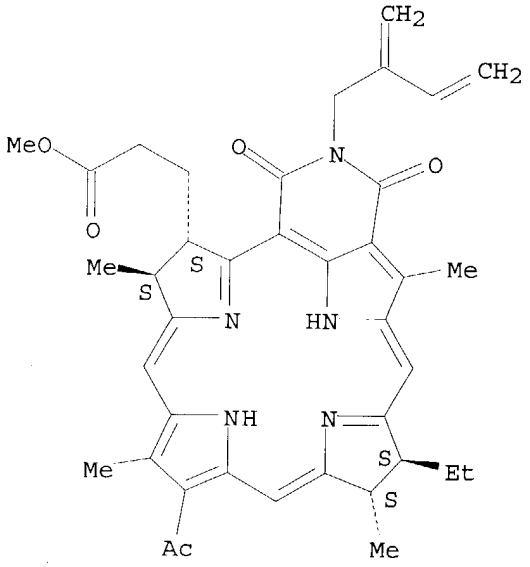


IT **478945-67-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction with C60 in synthesis of bacteriochlorin fullerene dyad)

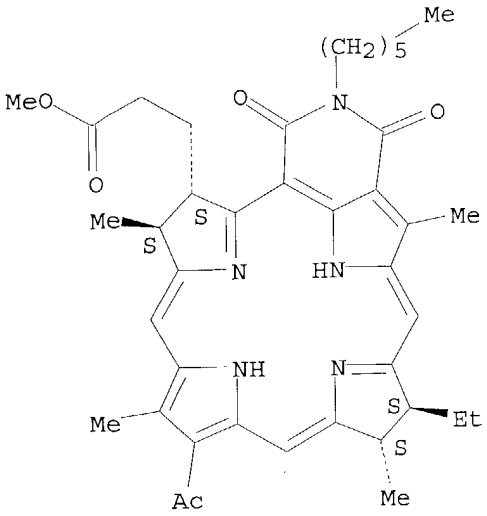
RN 478945-67-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-19-(2-methylene-3-butenyl)-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **438627-03-3**
RL: PRP (Properties)
(reference compound; photochem. and electrochem. properties of free base bacteriochlorin- and zinc chlorin-fullerene dyads)
RN 438627-03-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-1,5,6,15,16,18,19,20-octahydro-5-ethyl-19-hexyl-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:287224 HCAPLUS
DOCUMENT NUMBER: 137:63096
TITLE: Photophysical and Electrochemical Properties of New Bacteriochlorins and Characterization of Radical Cation and Radical Anion Species
AUTHOR(S): Fukuzumi, Shunichi; Ohkubo, Kei; Chen, Yihui; Pandey, Ravindra K.; Zhan, Riqiang; Shao, Jianguo; Kadish, Karl M.
CORPORATE SOURCE: Department of Material and Life Science, Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan
SOURCE: Journal of Physical Chemistry A (2002), 106(20), 5105-5113
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:63096

AB The synthesis, photophys., and photochem. properties of a series of stable bacteriochlorins containing a fused six-member anhydride or an imide ring are discussed. The Qy band (a1u → egx transition) in the near-IR region (NIR) lies between 788 and 831 nm depending upon the macrocycle substituents. Compds. with such a long-wavelength absorption are highly promising for their potential use in photodynamic therapy. Fluorescence maxima are also observed in the long-wavelength region of the spectrum, between 804 and 842 nm, and have lifetimes between 1.1 and 1.4 ns. The phosphorescence maxima are red-shifted to 840-870 nm. The triplet-triplet transient absorption spectra are observed to have maxima between 570 and 640 nm with lifetimes between 72 and 150 μs. The triplet excited states are efficiently quenched by oxygen to produce singlet oxygen. The quantum yields of the generated singlet oxygen were determined to be in the range of 0.33-0.55. The bacteriochlorin derivs. are easy to oxidize by one electron, and reversible half-wave potentials range between 0.65 and 0.82 V vs. SCE in benzonitrile containing 0.1 M tetra-n-butylammonium perchlorate (TBAP). The second oxidation is irreversible and occurs at a rather constant

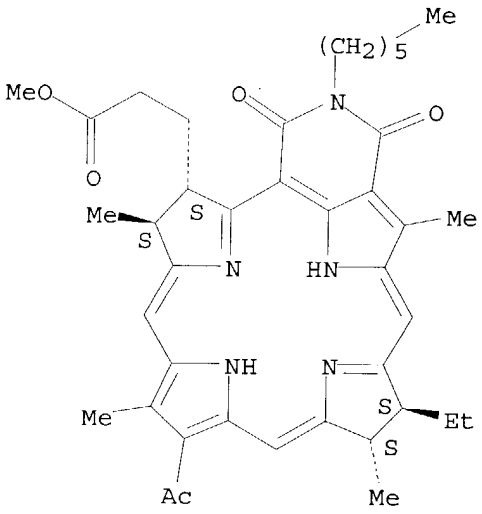
potential of 1.17-1.22 V independent of the macrocycle substituents. The bacteriochlorin derivs. are also easy to reduce, and the reversible first and second one-electron reduction potentials range between -0.53 and -0.80 V and between -0.95 and -1.28 V vs. SCE, resp. Spectroelectrochem. measurements reveal the expected π radical cation and π radical anion marker bands of the bacteriochlorin derivs. The ESR spectra of the radical cations and radical anions produced by the chemical oxidation and reduction
are reported, and the exptl. and calculated spin densities are compared to each other.

IT **438627-03-3P**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(intermediate/product/bacteriochlorin analog; preparation and photophys. and electrochem. properties of bacteriochlorin analogs containing fused 6-membered anhydride or imide ring in relation to photosensitizer use)

RN 438627-03-3 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-1,5,6,15,16,18,19,20-octahydro-5-ethyl-19-hexyl-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

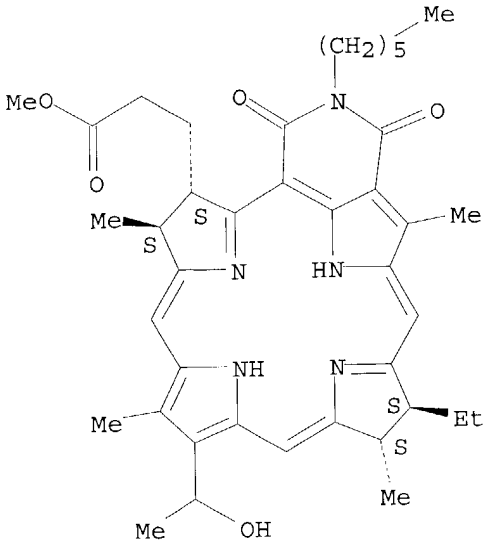


IT **438627-07-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation and photophys. and electrochem. properties of bacteriochlorin analogs containing fused 6-membered anhydride or imide ring in relation to photosensitizer use)

RN 438627-07-7 HCAPLUS

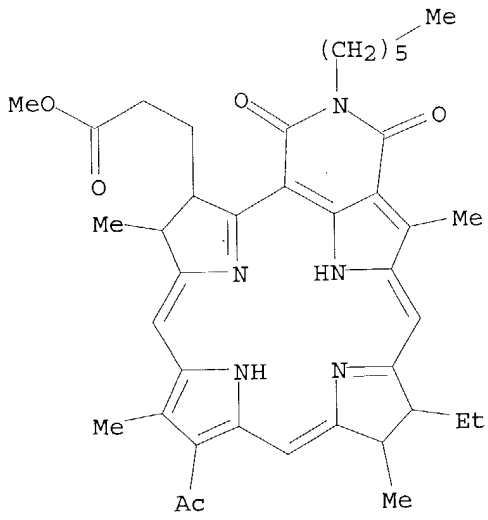
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-10-(1-hydroxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

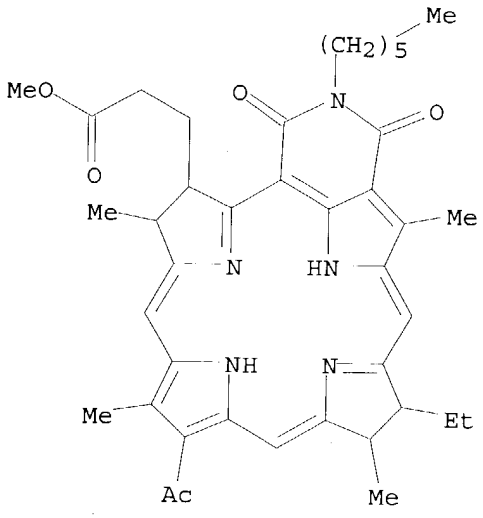


IT **439090-20-7 439097-71-9**
RL: PRP (Properties)
(photophys. properties of radical anions and cations of bacteriochlorin analogs containing fused 6-membered anhydride or imide ring)

RN 439090-20-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, radical ion(1-), (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)



RN 439097-71-9 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, radical ion(1+), (5S,6S,15S,16S)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:918882 HCAPLUS
DOCUMENT NUMBER: 136:37447
TITLE: Long wavelength absorbing bacteriochlorin alkyl ether analogs for the treatment and detection of hyperproliferative tissues such as tumors using photodynamic methods.
INVENTOR(S): Pandey, Ravindra K.; Dougherty, Thomas J.; Potter, William R.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1164136	A1	20011219	EP 2001-108984	20010411
EP 1164136	B1	20040609		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6624187	B1	20030923	US 2000-592150	20000612
CA 2342064	AA	20011212	CA 2001-2342064	20010321
AT 268777	E	20040615	AT 2001-108984	20010411
JP 2002020389	A2	20020123	JP 2001-116889	20010416
PRIORITY APPLN. INFO.:			US 2000-592150 A	20000612

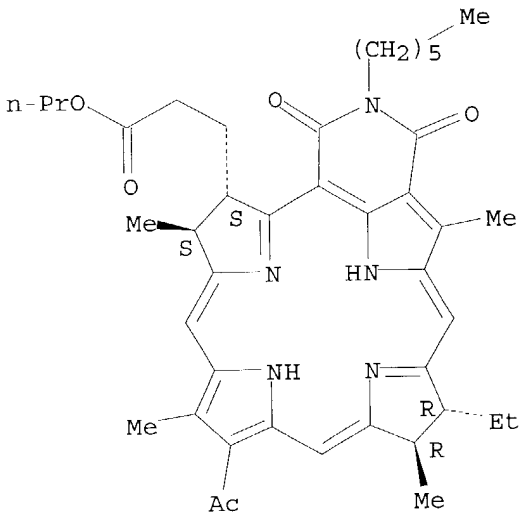
OTHER SOURCE(S): MARPAT 136:37447
AB Novel compds. I [R1, R5, R9, R10 = independently C1-C3 alkyl (provided that at least 3 = Me); R2 = OH, OR11, NHR11, aryl or amino acid; R3, R4 = independently C(O)R11 or taken together = C(O)NR12C(O); R6, R7 = independently C1-C3; R8 = O-alkyl or S-alkyl, aryl or heterocyclic ring; R11 = C1-C6 alkyl; R12 = C1-C12 alkyl, aryl or aminoalkyl (C1-C8); provided that at least one of R8, R11, and R12 is hydrophobic and together

contain at least 10 carbon atoms] that either preferentially absorb into hyperproliferative tissue and absorb light efficiently at a wavelength of between about 700 and about 850 nm or act as intermediates for such absorbing compds were prepared Thus, 3-deacetyl-3-(1-heptyloxyethyl)-bacteriopurpurin-N-hexylimide Pr ester (II) was prepared in 6 or 7 steps from bacteriochlorophyll A. The in vivo photosensitizing efficacy of II against a mouse tumor model system (RIF tumor) was evaluated. The invention also includes method of making and using the compds.

IT **182253-28-7P 380229-03-8P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(long wavelength absorbing bacteriochlorin alkyl ether analogs)

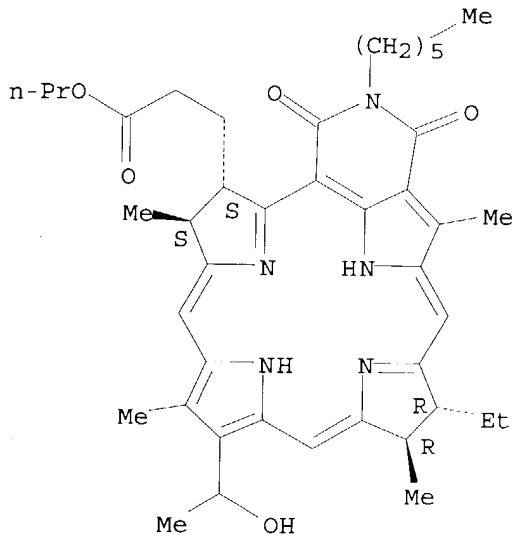
RN 182253-28-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



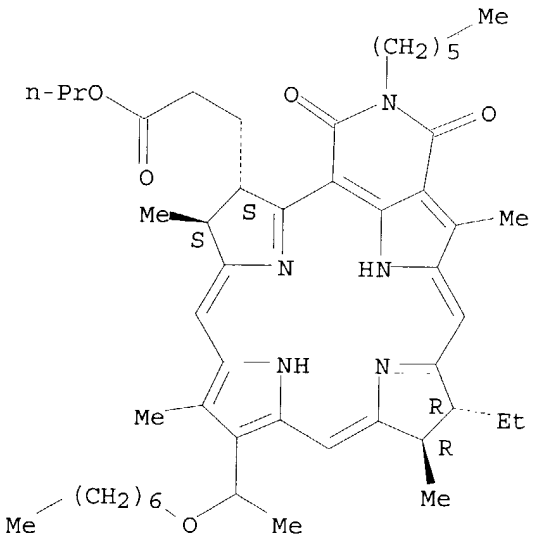
RN 380229-03-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-7H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-10-(1-hydroxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **380229-05-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(long wavelength absorbing bacteriochlorin alkyl ether analogs)
RN 380229-05-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-7H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(heptyloxy)ethyl]-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

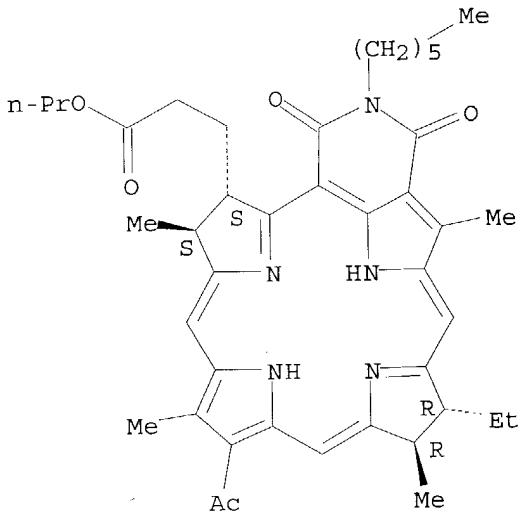
ACCESSION NUMBER: 2001:909501 HCAPLUS
DOCUMENT NUMBER: 136:179872
TITLE: Bacteriopurpurinimides: Highly Stable and Potent Photosensitizers for Photodynamic Therapy
AUTHOR(S): Chen, Yihui; Graham, Andrew; Potter, William; Morgan, Janet; Vaughan, Lurine; Bellnier, David A.; Henderson, Barbara W.; Oseroff, Allan; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: Photodynamic Therapy Center and Department of Dermatology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(2), 255-258
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The in situ conversion of the unstable bacteriochlorophyll a present in Rhodobacter sphaeroides produced highly stable bacteriopurpurin-18 which in a sequence of reactions was converted into a series of alkyl ether analogs of bacteriopurpurin-18-N-alkylimides with long wavelength absorption near 800 nm. The effective photosensitizers were found to localize in mitochondria but did not show any specific displacement of 3H-PK11195, suggesting that the mitochondrial peripheral benzodiazepine receptor is not the cellular binding site for this class of compds. The heptyl ether analog of bacteriopurpurin-18 showed excellent PDT efficacy in mice with implanted with fibrosarcoma cells.

IT **182253-28-7P 380229-03-8P 380229-05-0P**
400604-82-2P 400604-83-3P 400604-84-4P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of and photosensitizing efficacy of bacteriopurpurin-18 analogs against fibrosarcoma)

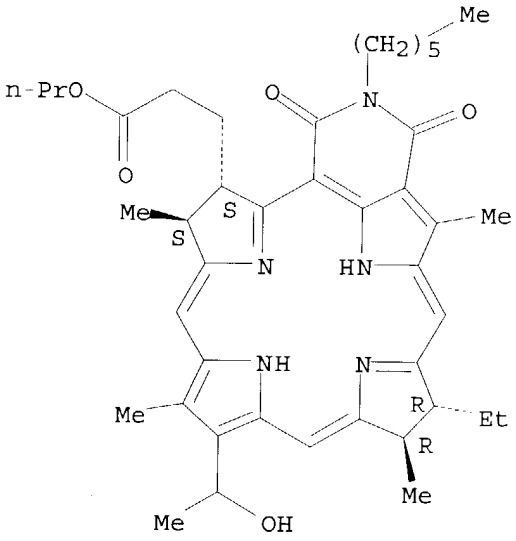
RN 182253-28-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



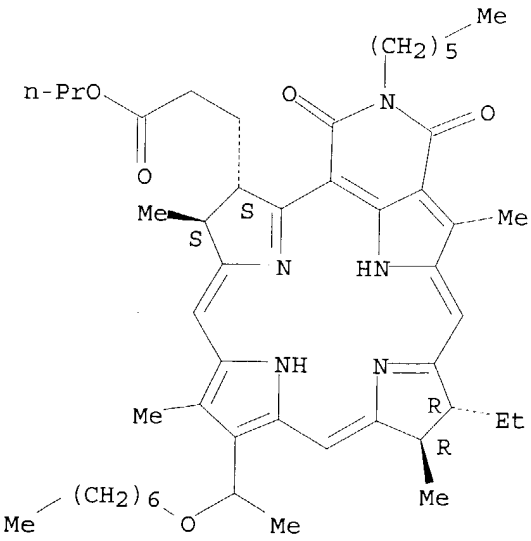
RN 380229-03-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-7H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-10-(1-hydroxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 380229-05-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-7H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(heptyloxy)ethyl]-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

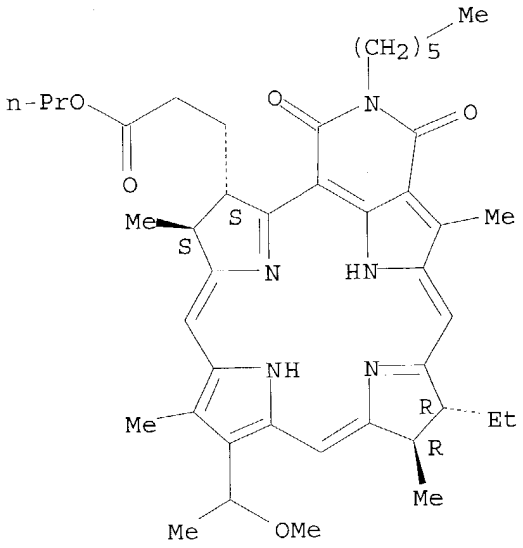
Absolute stereochemistry.



RN 400604-82-2 HCAPLUS

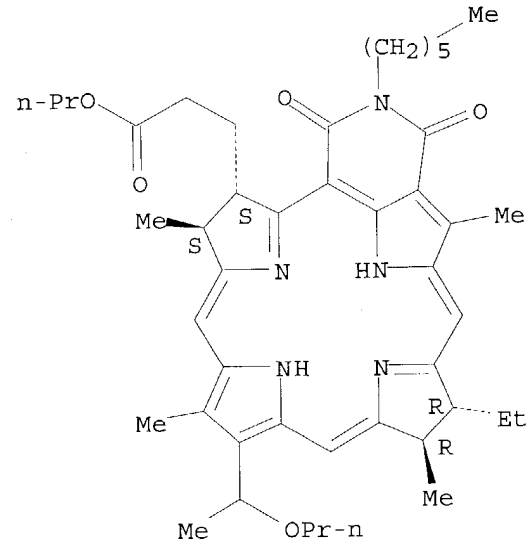
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 400604-83-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

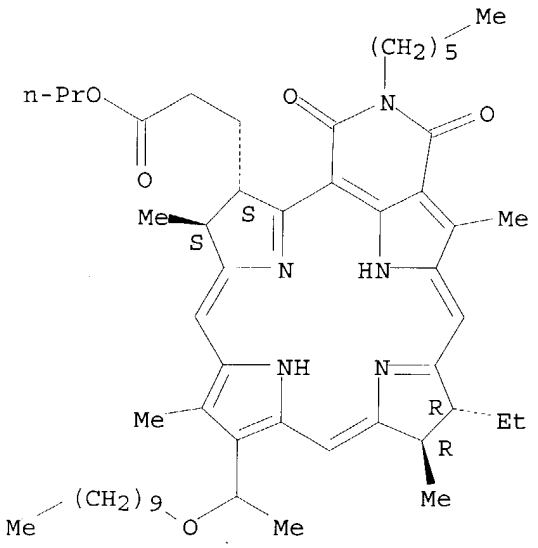
Absolute stereochemistry.



RN 400604-84-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-

b]azacyclononadecine-16-propanoic acid, 10-[1-(decyloxy)ethyl]-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:472002 HCAPLUS
DOCUMENT NUMBER: 135:70116
TITLE: Preparation of chlorin and bacteriochlorin-based aminophenyl-modified diethylenetriaminepentaacetic acid (DTPA) and N2S2 conjugates for MRI contrast media and radiopharmaceuticals
INVENTOR(S): Pandey, Ravindra K.; Grossman, Zachary; Kanter, Peter; Dougherty, Thomas J.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1110963	A2	20010627	EP 2000-128019	20001220
EP 1110963	A3	20011219		
EP 1110963	B1	20040421		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2001046983	A1	20011129	US 2000-739155	20001218
US 6534040	B2	20030318		
AT 264862	E	20040515	AT 2000-128019	20001220
JP 2001335578	A2	20011204	JP 2000-404615	20001225
PRIORITY APPLN. INFO.:			US 1999-171961P P	19991223

US 2000-739155 A 20001218

OTHER SOURCE(S): MARPAT 135:70116

AB Claimed are compns. that are a chemical combination of porphyrins, chlorins, bacteriochlorins, and related tetra-pyrrolic compds. with radioactive elements such as Tc99, Gd, In111 and radioactive iodine. The invention includes certain chlorin and bacteriochlorin-based bisaminoethanethiol (N2S2) and aminophenyl-modified diethylenetriaminepentaacetic acid (DTPA) conjugates. Example compds. include a Gd(III) chelate of HPPH-aminophenylDTPA conjugate compound with a pheophorbide derivative, I, or a Gd(III) chelate of the purpurin-18-imide analog II, among others. When the radioactive element can form cations, the compound is usually a chelate with the porphyrin or chlorin structure. When the element forms anions, the compound is usually a direct chemical combination of the radioactive element into the porphyrin or chlorin structure. The invention further includes the method of using the compds. of the invention for diagnostic imaging of hyperproliferative tissue such as tumors and new blood vessel growth as is associated with the wet form of age-related macular degeneration. The invention further includes methods of making the compds. Compds. for MRI contrast imaging of the invention are usually Tc99, In111 or Gd(III) complexes of compds. of the invention.

IT **346432-58-4P**

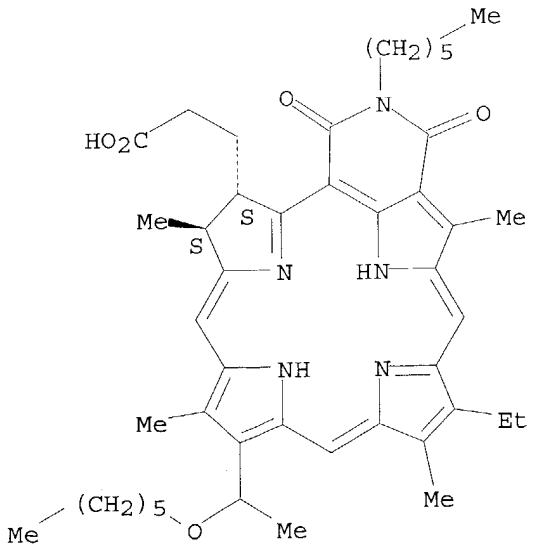
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coupling with aminophenyl-modified diethylenetriaminepentaacetate for preparation of MRI contrast agent)

RN 346432-58-4 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **346432-55-1P**

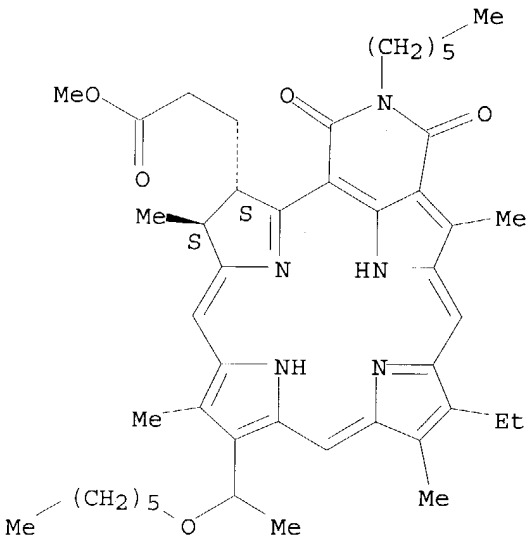
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of esters to acids)

RN 346432-55-1 HCAPLUS

CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L18 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:312519 HCAPLUS
DOCUMENT NUMBER: 135:76709
TITLE: Synthesis, Photophysical Properties, Tumor Uptake, and Preliminary in Vivo Photosensitizing Efficacy of a Homologous Series of 3-(1'-Alkyloxy)ethyl-3-devinylpurpurin-18-N-alkylimides with Variable Lipophilicity
AUTHOR(S): Zheng, Gang; Potter, William R.; Camacho, Susan H.; Missert, Joseph R.; Wang, Guosheng; Bellnier, David A.; Henderson, Barbara W.; Rodgers, Michael A. J.; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: Photodynamic Therapy Center Department of Nuclear Medicine/Radiology, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(10), 1540-1559
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:76709

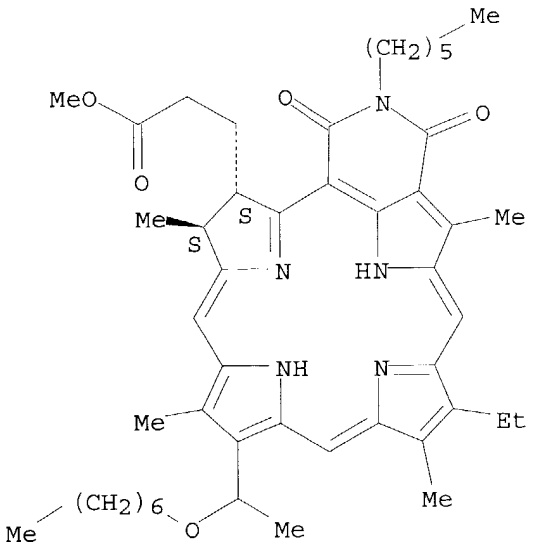
AB Starting from methylpheophorbide-a, a homologous series of purpurinimides containing alkyl substituents at two different positions [as 3-(11-O-alkyl) and 132-N-alkyl] were synthesized. These compds. with variable lipophilicity (log P 5.32-16.44) exhibit long wavelength absorption near λmax700 nm (ε: 45 000 in dichloromethane) with singlet oxygen (1O2) production in the range of 57-60%. The shifts in in vivo absorptions and tumor/skin uptake of these compds. were determined in C3H mice bearing RIF tumors by in vivo reflectance spectroscopy. The results

obtained from a set of photosensitizers with similar lipophilicity (log P 10.68-10.88) indicate that besides the overall lipophilicity, the presence and position of the alkyl groups (O-alkyl vs N-alkyl) in a mol. play an important role in tumor uptake, tumor selectivity, and in vivo PDT efficacy. At present, all purpurinimide analogs are being evaluated at various doses, and expts. are underway to establish a quant. structure-activity relationship on a limited set of compds. The 1D and 2D NMR and mass spectrometry analyses confirmed the structures of the desired purpurinimides and the byproducts formed during various reaction conditions. The mechanisms of the formation of the unexpected 12-formyl- and 12-(hydroxymethyl)purpurinimides under certain reaction conditions are also discussed.

IT **291293-52-2P 346432-55-1P 347142-33-0P**
347142-35-2P 347142-39-6P 347142-40-9P
347142-41-0P 347142-43-2P 347142-45-4P
347142-47-6P 347142-48-7P 347142-49-8P
347142-50-1P 347142-54-5P 347142-56-7P
347142-57-8P 347142-58-9P 347142-59-0P
347142-60-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis, photophys. properties, tumor uptake, and preliminary in vivo photosensitizing efficacy of a homologous series of 3-(1'-alkyloxy)ethyl-3-devinylpurpurin-18-N-alkylimides with variable lipophilicity)

RN 291293-52-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(heptyloxy)ethyl]-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

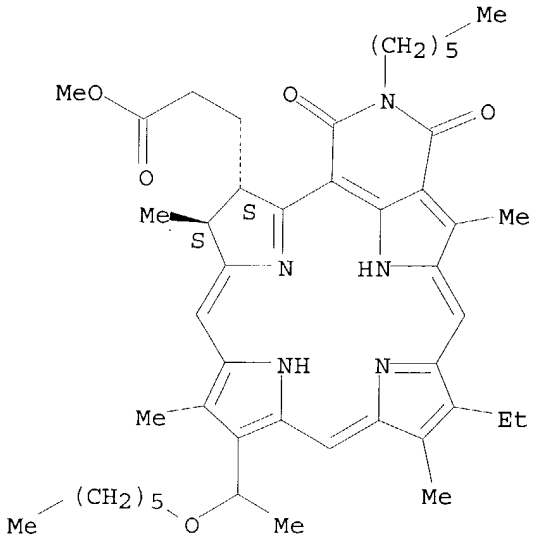
Absolute stereochemistry.



RN 346432-55-1 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-

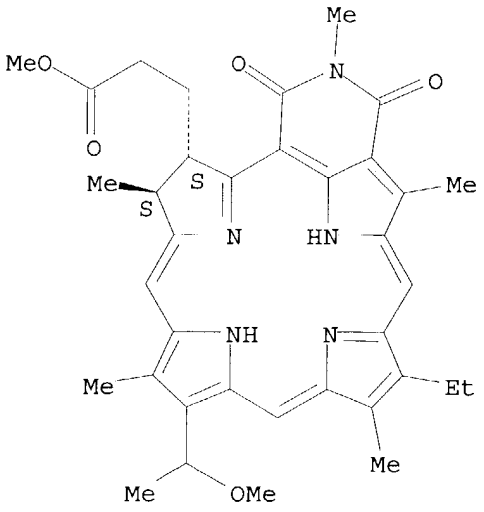
(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



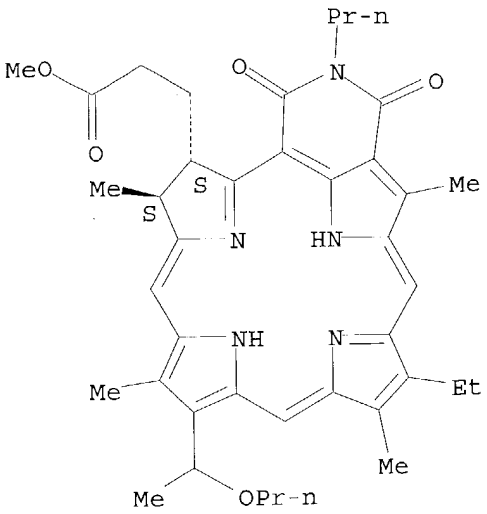
RN 347142-33-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-1,15,16,18,19,20-hexahydro-10-(1-methoxyethyl)-6,11,15,19,22-pentamethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



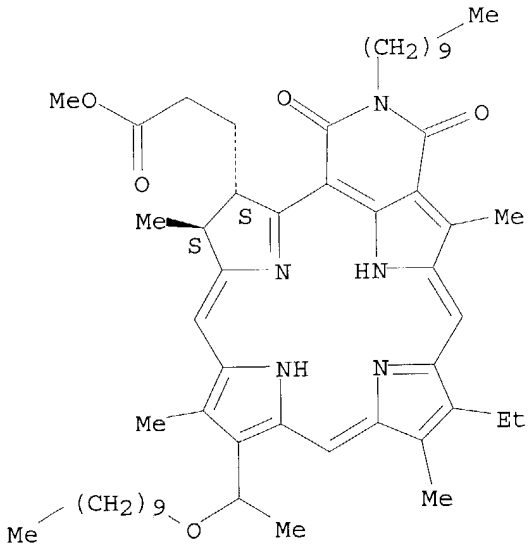
RN 347142-35-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



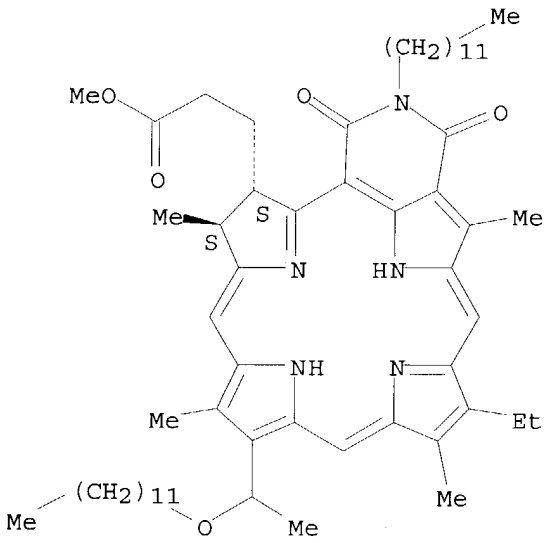
RN 347142-39-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-decyl-10-[1-(decyloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



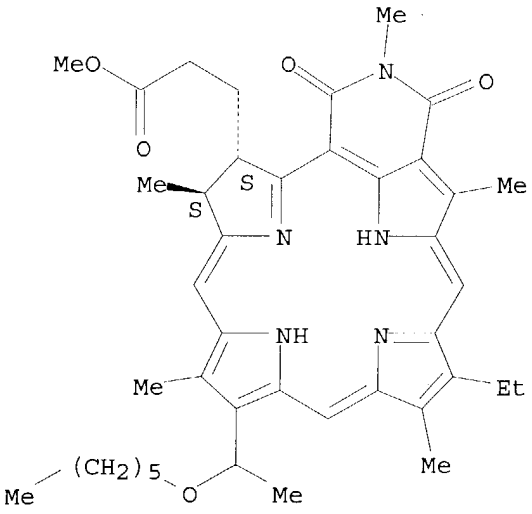
RN 347142-40-9 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-dodecyl-10-[1-(dodecyloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



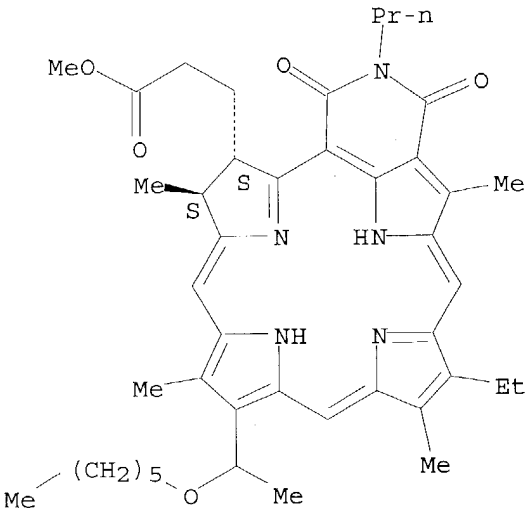
RN 347142-41-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,19,22-pentamethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



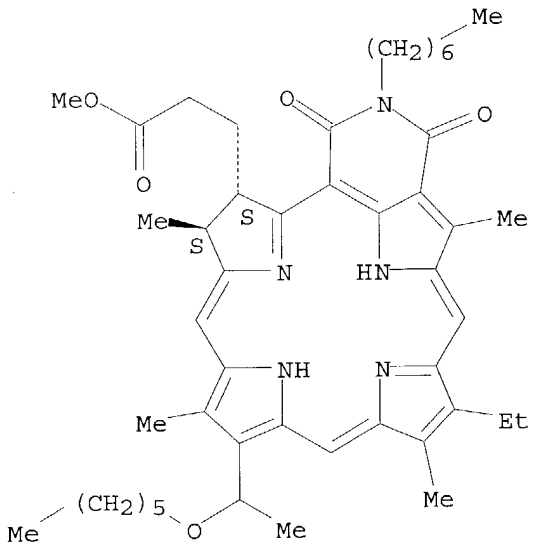
RN 347142-43-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



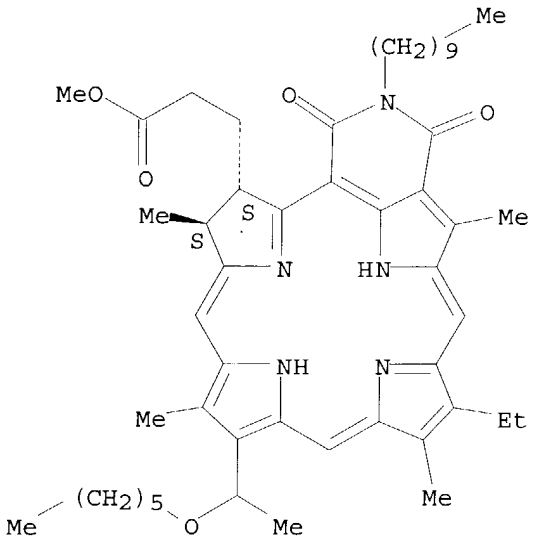
RN 347142-45-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-heptyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



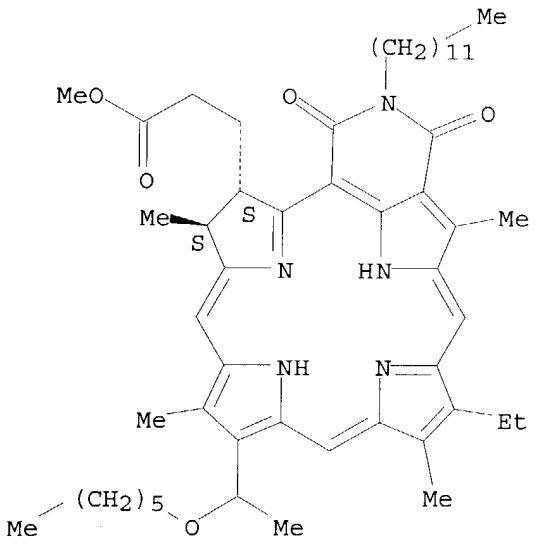
RN 347142-47-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-decyl-5-ethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



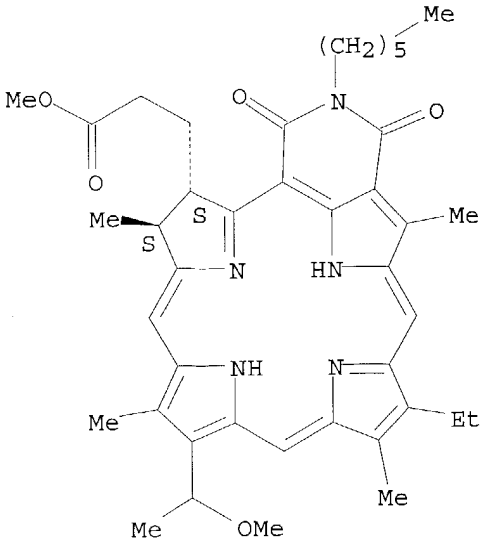
RN 347142-48-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-dodecyl-5-ethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



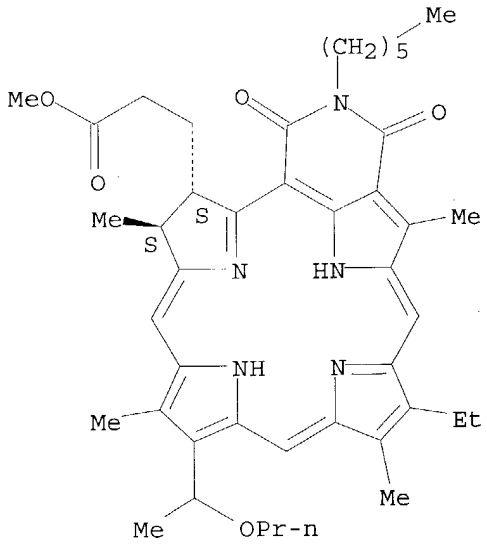
RN 347142-49-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



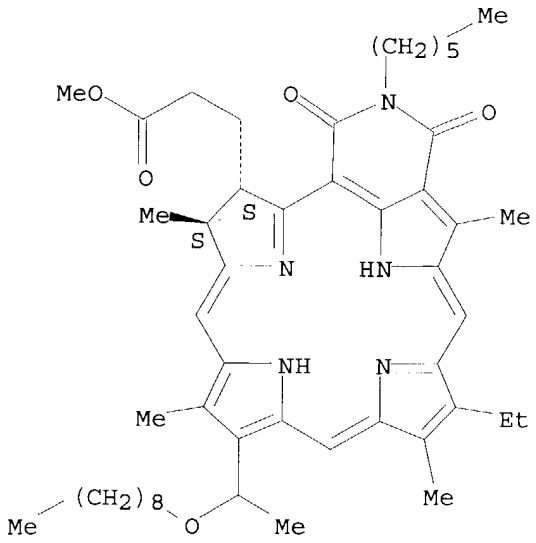
RN 347142-50-1 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



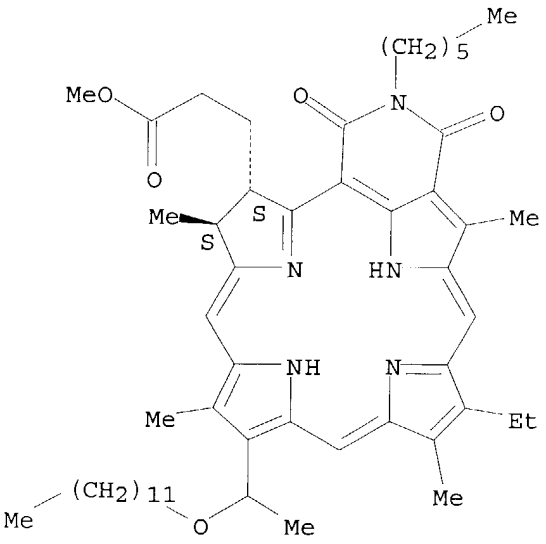
RN 347142-54-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-10-[1-(nonyloxy)ethyl]-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



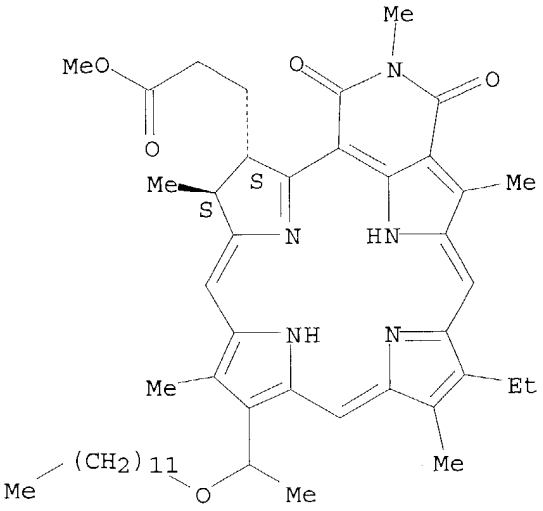
RN 347142-56-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-(dodecyloxy)ethyl]-5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



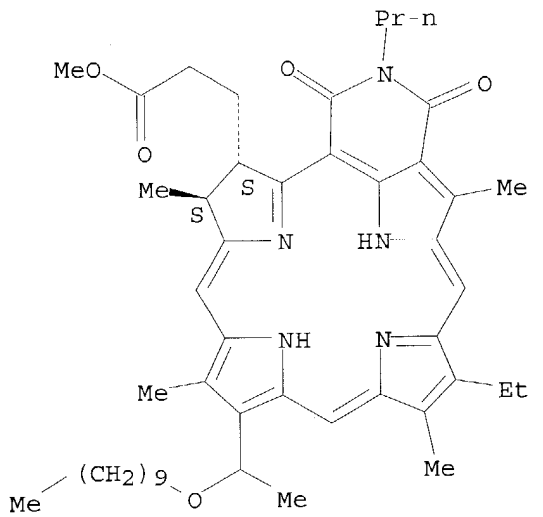
RN 347142-57-8 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-(dodecyloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,19,22-pentamethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



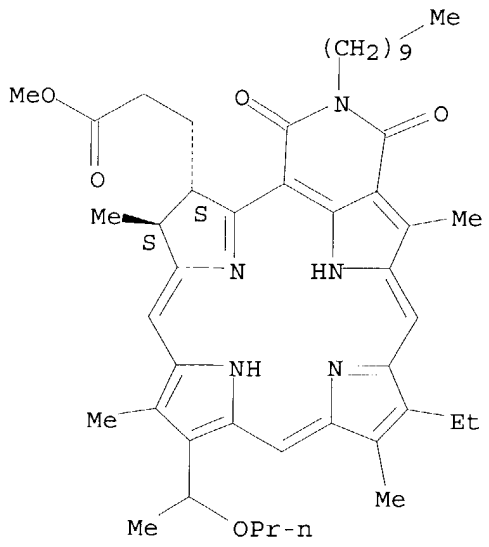
RN 347142-58-9 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-(decyloxy)ethyl]-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



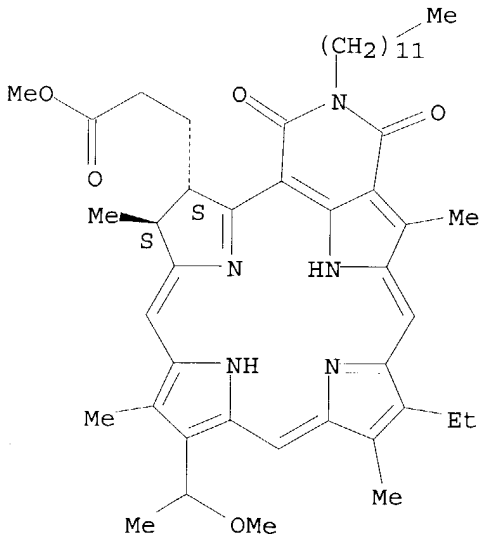
RN 347142-59-0 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-decyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 347142-60-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-dodecyl-5-ethyl-1,15,16,18,19,20-hexahydro-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

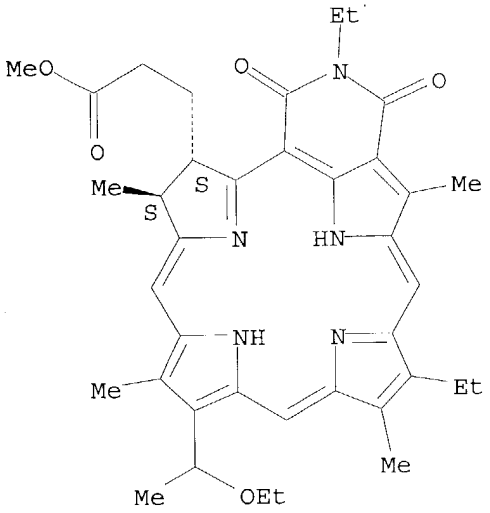
Absolute stereochemistry.



IT **347142-34-1P 347142-36-3P 347142-37-4P**
347142-38-5P 347142-42-1P 347142-44-3P
347142-46-5P 347142-51-2P 347142-52-3P
347142-53-4P 347142-55-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis, photophys. properties, tumor uptake, and preliminary in vivo photosensitizing efficacy of a homologous series of 3-(1'-alkyloxy)ethyl-3-devinylpurpurin-18-N-alkylimides with variable lipophilicity)

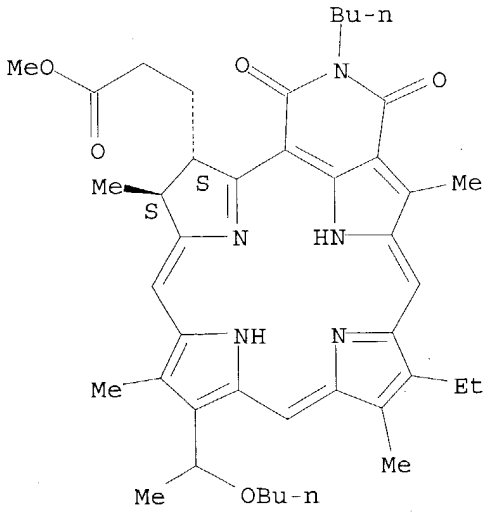
RN 347142-34-1 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-(1-ethoxyethyl)-5,19-diethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 347142-36-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-(1-butoxyethyl)-19-butyl-5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

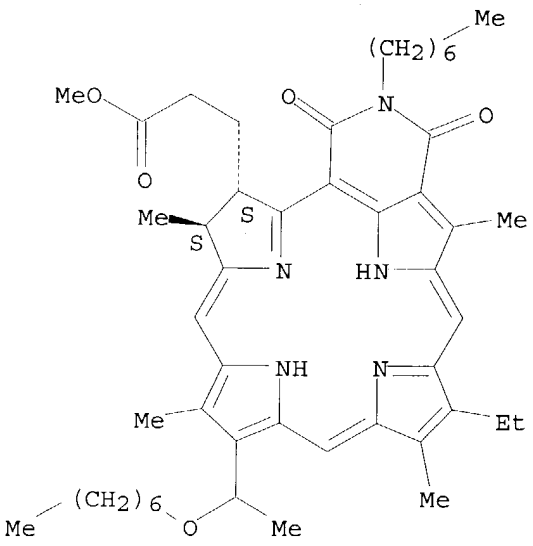
Absolute stereochemistry.



RN 347142-37-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-heptyl-10-[1-

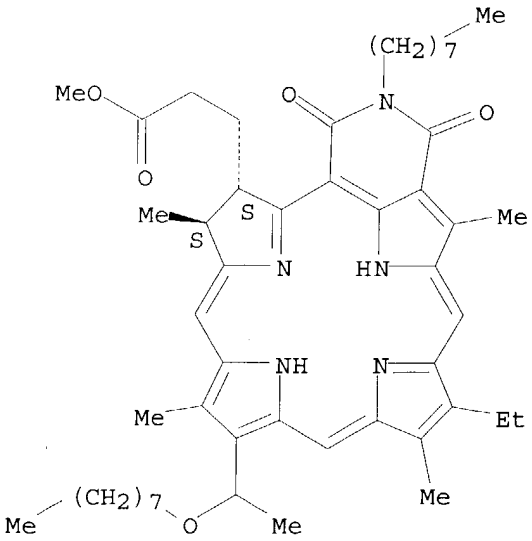
(heptyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 347142-38-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-19-octyl-10-[1-(octyloxy)ethyl]-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

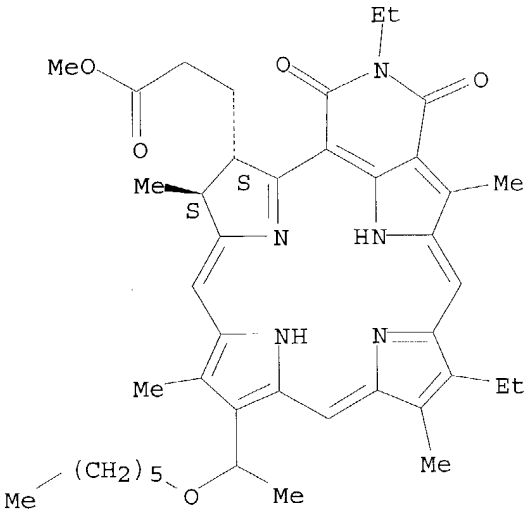
Absolute stereochemistry.



RN 347142-42-1 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5,19-diethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-

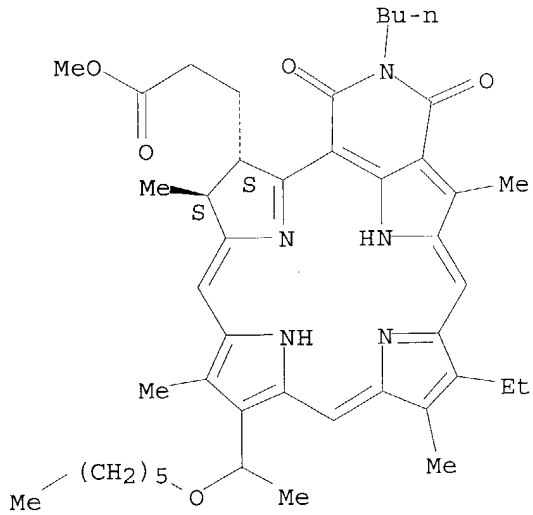
dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



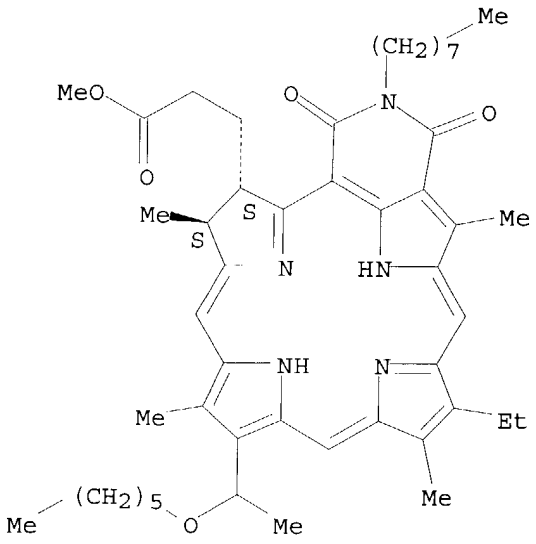
RN 347142-44-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 19-butyl-5-ethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



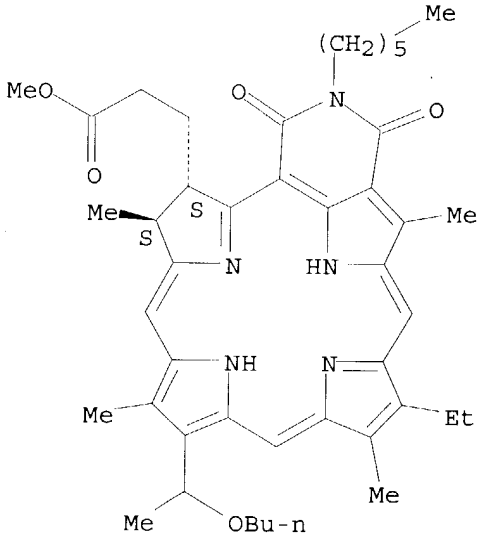
RN 347142-46-5 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(hexyloxy)ethyl]-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-19-octyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



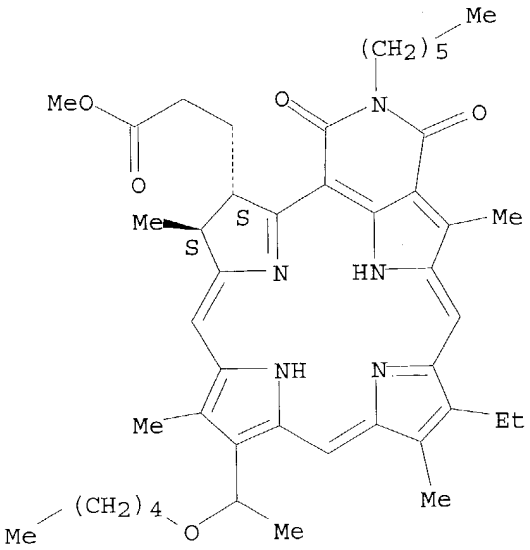
RN 347142-51-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-(1-butoxyethyl)-5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



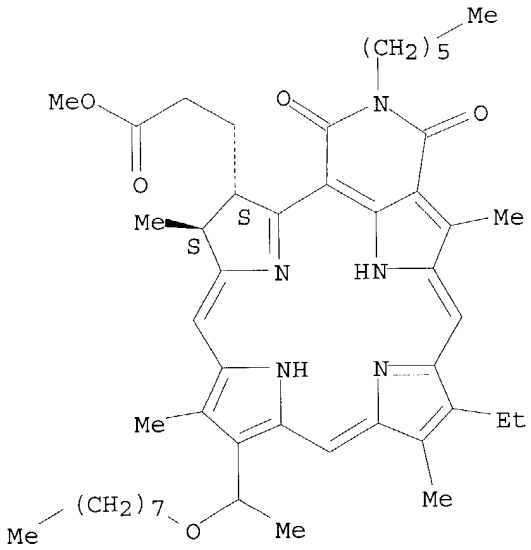
RN 347142-52-3 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-[1-(pentyloxy)ethyl]-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



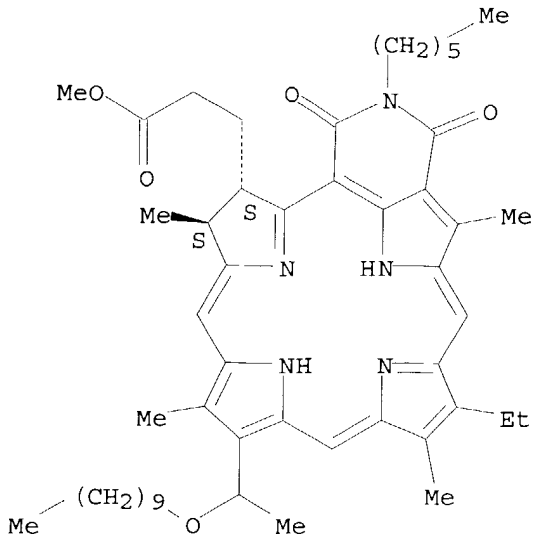
RN 347142-53-4 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-10-[1-(octyloxy)ethyl]-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



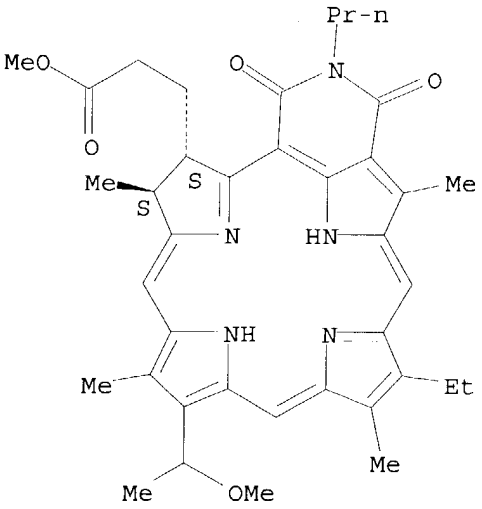
RN 347142-55-6 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-(decyloxy)ethyl]-5-ethyl-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **347142-69-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis, photophys. properties, tumor uptake, and preliminary in vivo photosensitizing efficacy of a homologous series of 3-(1'-alkyloxy)ethyl-3-devinylpurpurin-18-N-alkylimides with variable lipophilicity)
RN 347142-69-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-1,15,16,18,19,20-hexahydro-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN

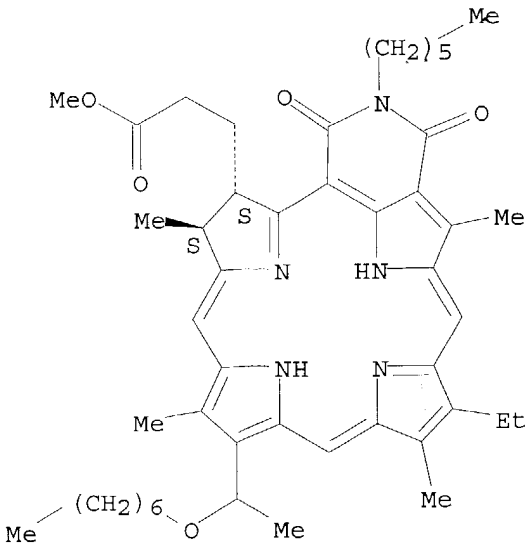
ACCESSION NUMBER: 2000:458495 HCAPLUS
DOCUMENT NUMBER: 133:222479
TITLE: Purpurinimides as photosensitizers: effect of the presence and position of the substituents in the in vivo photodynamic efficacy
AUTHOR(S): Rungta, Ankur; Zheng, Gang; Missert, Joseph R.; Potter, William R.; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: Photodynamic Therapy Center, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(13), 1463-1466
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:222479

AB This study presents a novel approach for the regioselective synthesis of a series of alkyl ether analogs of purpurin-18-N-alkylimide. In the purpurinimide series, this is the first example which demonstrates that the presence and position of the substituents in the macrocycle makes a remarkable difference in the in vivo PDT efficacy.

IT **291293-52-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(effect of the presence and position of the substituents in the in vivo photodynamic efficacy of purpurinimides as photosensitizers)

RN 291293-52-2 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(heptyloxy)ethyl]-19-hexyl-1,15,16,18,19,20-hexahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

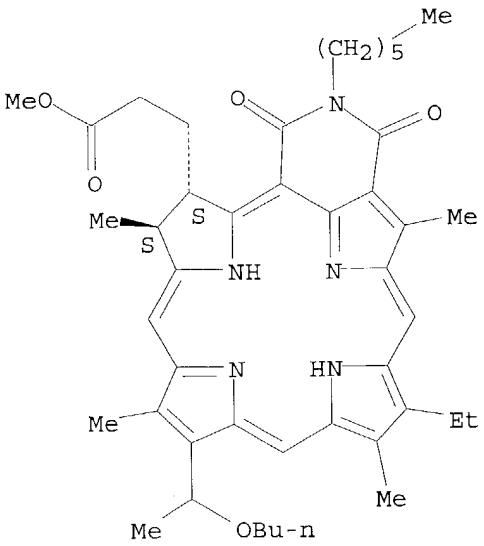
L18 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:94004 HCAPLUS
DOCUMENT NUMBER: 132:248051
TITLE: Photosensitizers related to purpurin-18-N-alkylimides: a comparative in vivo tumoricidal ability of ester versus amide functionalities
AUTHOR(S): Zheng, Gang; Potter, William R.; Sumlin, Adam; Dougherty, Thomas J.; Pandey, Ravindra K.
CORPORATE SOURCE: Photodynamic Therapy Center, Roswell Park Cancer Institute, Buffalo, NY, 14263, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(2), 123-127
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB For a comparative study, 3-(alkyloxyethyl)-3-devinylpurpurin-18-N-hexylimides with ester and amide functionalities were investigated for tumor selectivity and in vivo photosensitizing efficacy. Compared to amide analogs, the related photosensitizers with ester functionalities were found to be more effective. Among these compds. the 3-devinyl-(3-hexyloxyethyl)-purpurin-18-N-hexylimide as Me ester 12 showed excellent tumor uptake (tumor vs. muscle ratio: 8:1), and produced 100% tumor cure on day 30 at a dose of 1.0 μmol/kg. The mice were treated with light (135 J/cm2, 705 nm) at 24 h post injection of the drug.

IT **262617-02-7P 262617-03-8P 262617-04-9P**
262617-05-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(photosensitizers related to purpurin-18-N-alkylimides: comparative antitumor action of ester vs. amide functionalities)

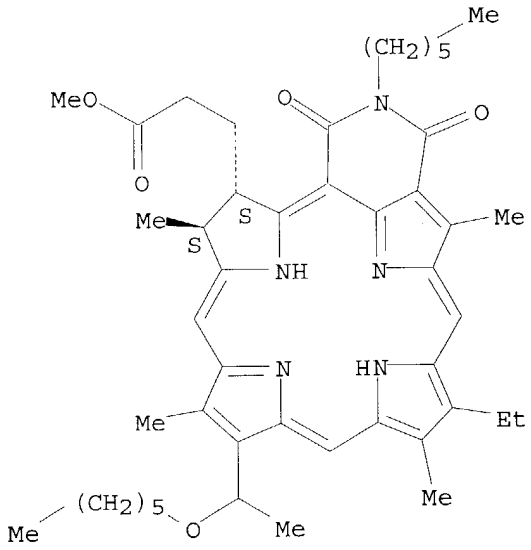
RN 262617-02-7 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-(1-butoxyethyl)-5-ethyl-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



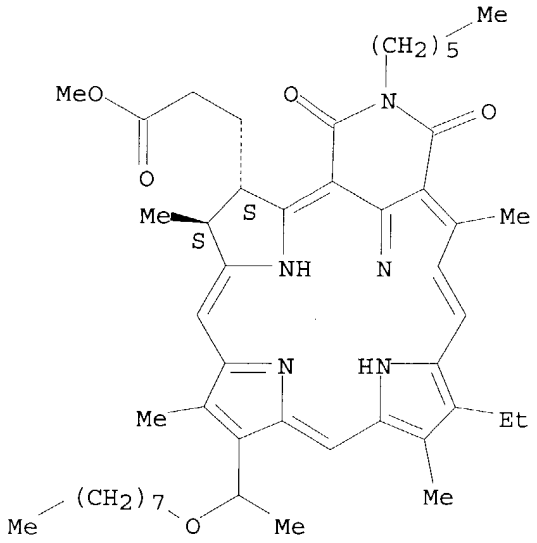
RN 262617-03-8 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-10-[1-(hexyloxy)ethyl]-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



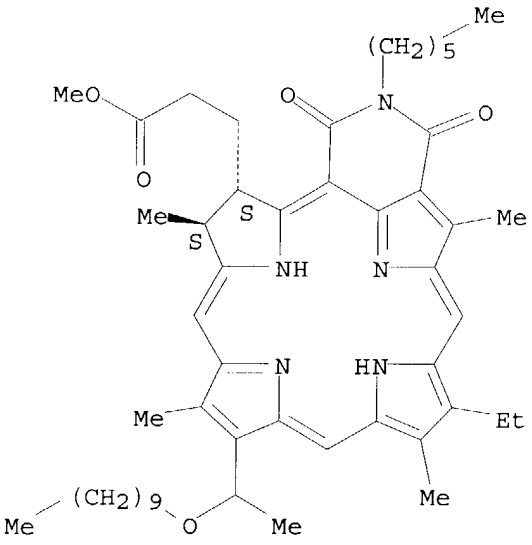
RN 262617-04-9 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-10-[1-(octyloxy)ethyl]-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 262617-05-0 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-[1-(decyloxy)ethyl]-5-ethyl-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:819376 HCAPLUS
DOCUMENT NUMBER: 132:61276
TITLE: Carotene analog of porphyrins, chlorins and

bacteriochlorins as therapeutic and diagnostic agents
INVENTOR(S): Pandey, Ravindra K.; Potter, William R.; Dougherty, Thomas J.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9967248	A1	19991229	WO 1999-US12170	19990601
W: CA, MX, NO				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6103751	A	20000815	US 1998-102417	19980622
CA 2331763	AA	19991229	CA 1999-2331763	19990601
EP 1087974	A1	20010404	EP 1999-957165	19990601
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NO 2000006543	A	20010214	NO 2000-6543	20001221

PRIORITY APPLN. INFO.: US 1998-102417 A 19980622
WO 1999-US12170 W 19990601

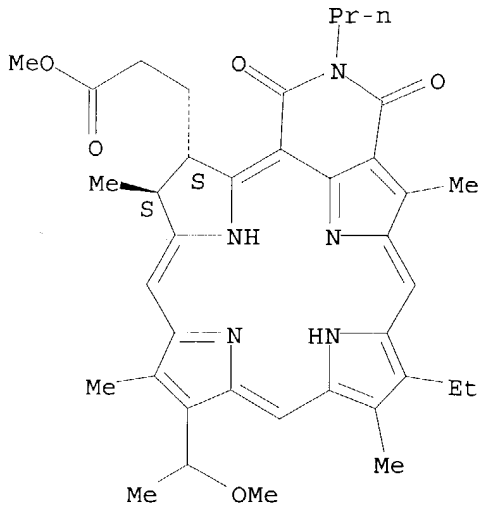
OTHER SOURCE(S): MARPAT 132:61276

AB Photodynamic compds. are described which have desired photodiagnostic qualities but with reduced photosensitizing side effects. Such compds. are carotene conjugates of photosensitizers selected from the group consisting of porphyrins, chlorins and bacteriochlorins. In examples given, carotene conjugates of HPPH and a fused imide ring purpurin were significantly taken up by fibrosarcoma tumors in mice when compared to the parent compds. Due to their strong fluorescence and higher uptake in tumors, such compds. show great potential for use as diagnostic agents for malignant and non-malignant tumors. Preliminary photodynamic antitumor activities of some compds. are also reported.

IT **241802-95-9P 241802-96-0P 241802-97-1P**
241802-98-2P 241802-99-3P 241803-00-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(carotene analog of porphyrins, chlorins and bacteriochlorins as therapeutic and diagnostic agents)

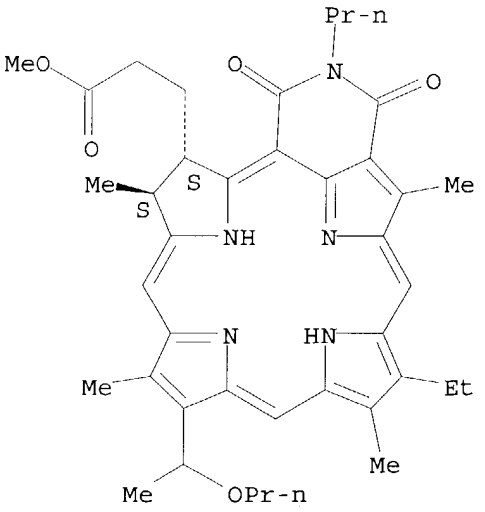
RN 241802-95-9 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 16,18,19,20-tetrahydro-5-ethyl-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



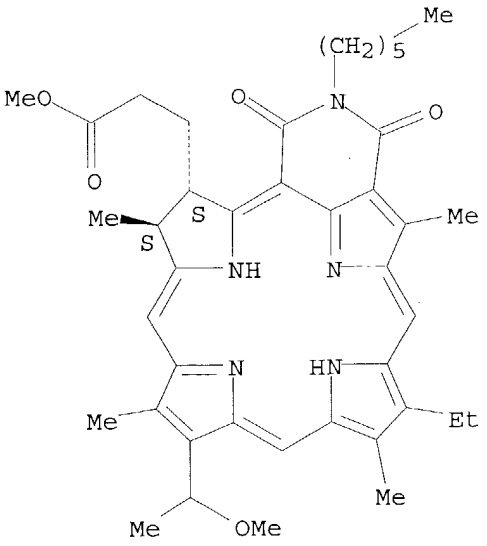
RN 241802-96-0 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



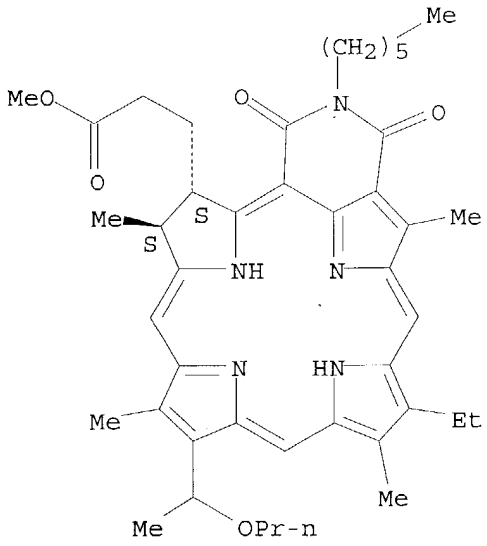
RN 241802-97-1 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-16,18,19,20-tetrahydro-10-(1-methoxyethyl)-6,10,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



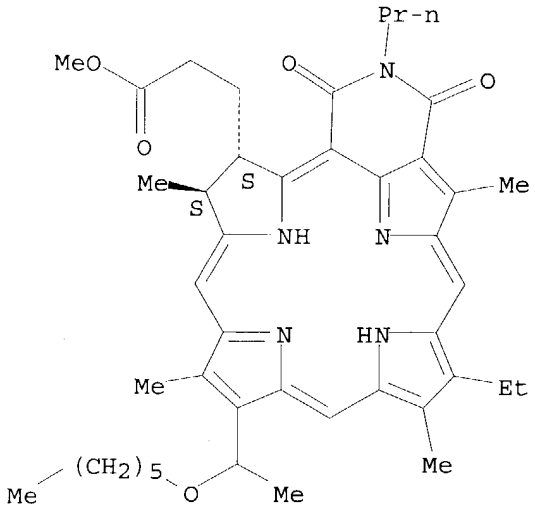
RN 241802-98-2 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



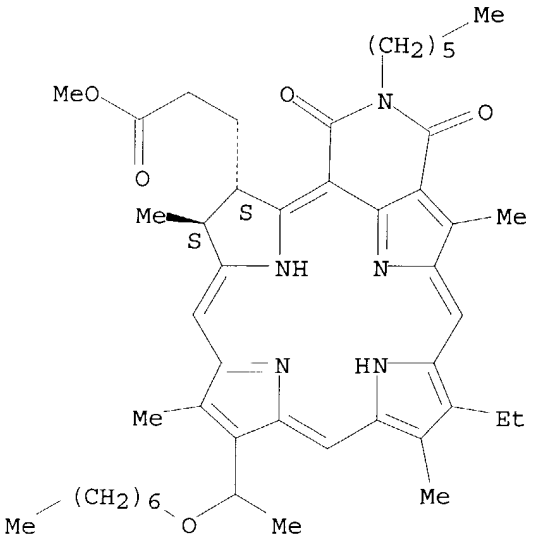
RN 241802-99-3 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(hexyloxy)ethyl]-16,18,19,20-tetrahydro-6,111,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 241803-00-9 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(heptyloxy)ethyl]-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:582655 HCAPLUS
DOCUMENT NUMBER: 131:199558
TITLE: synthesis and antitumor activity of alkyl ether analogs of chlorins having an N-substituted imide ring

INVENTOR(S): Pandey, Ravindra K.; Potter, William R.; Dougherty, Thomas J.
PATENT ASSIGNEE(S): Health Research, Inc., USA
SOURCE: U.S., 7 pp., Cont.-in-part of U.S. 5,864,035.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5952366	A	19990914	US 1998-102394	19980622
US 5770730	A	19980623	US 1996-613134	19960308
US 5864035	A	19990126	US 1997-812029	19970306
CA 2335514	AA	19991229	CA 1999-2335514	19990305
WO 9967249	A1	19991229	WO 1999-US4924	19990305
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1090006	A1	20010411	EP 1999-909878	19990305
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

PRIORITY APPLN. INFO.:

US 1996-613134	A2	19960308
US 1997-812029	A2	19970306
US 1998-102394	A	19980622
WO 1999-US4924	W	19990305

OTHER SOURCE(S): MARPAT 131:199558

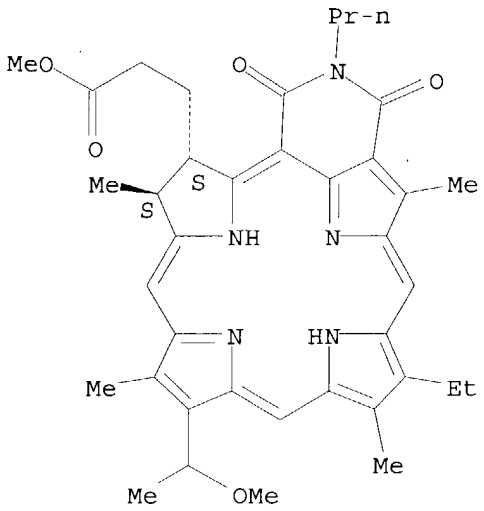
AB Synthesis and antitumor activity of alkyl ether analogs of chlorins having an N-substituted imide ring (I) (R1,R2 = alkyl together containing at least six carbon atoms; R3 = alkyl) is presented. I have utility in photodynamic therapy in treatment of tumors and other diseases. The invention includes a method of treatment by contacting a tumor with the compound and then exposing the tumor to light.

IT **241802-95-9P 241802-96-0P 241802-97-1P**
241802-98-2P 241802-99-3P 241803-00-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and antitumor activity of alkyl ether analogs of chlorins having an N-substituted imide ring)

RN 241802-95-9 HCAPLUS

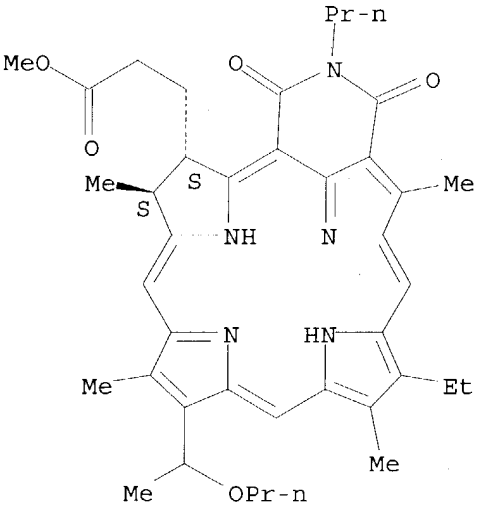
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 16,18,19,20-tetrahydro-5-ethyl-10-(1-methoxyethyl)-6,11,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



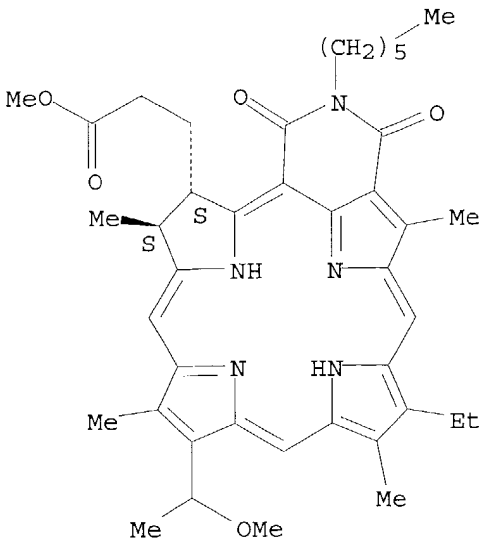
RN 241802-96-0 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



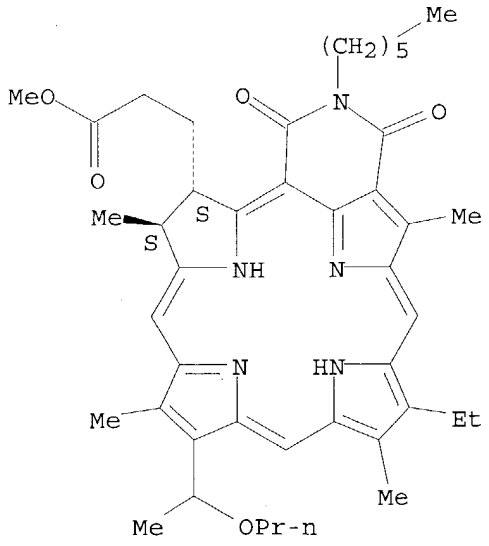
RN 241802-97-1 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-16,18,19,20-tetrahydro-10-(1-methoxyethyl)-6,10,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



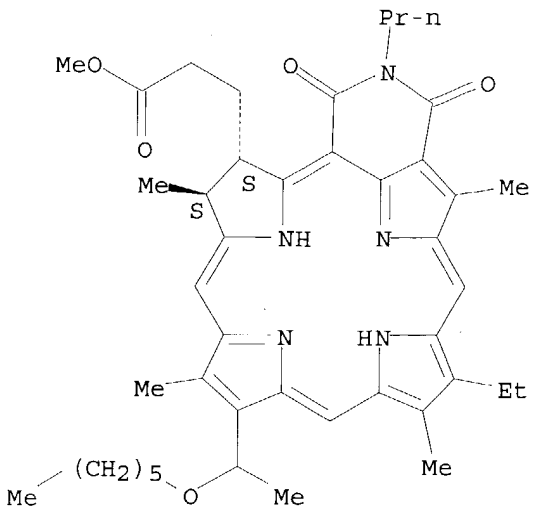
RN 241802-98-2 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-10-(1-propoxyethyl)-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



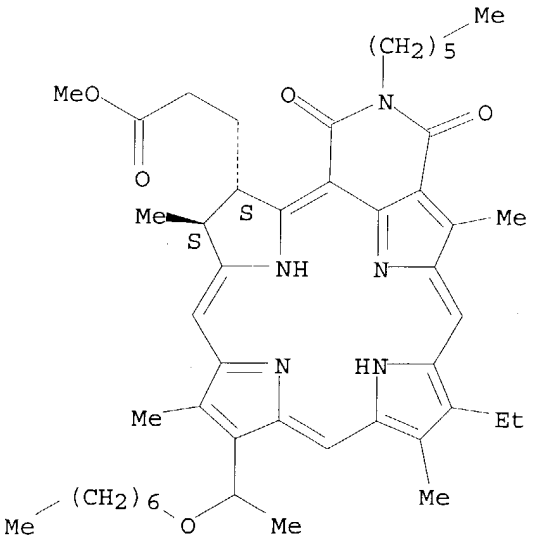
RN 241802-99-3 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(hexyloxy)ethyl]-16,18,19,20-tetrahydro-6,111,15,22-tetramethyl-18,20-dioxo-19-propyl-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 241803-00-9 HCAPLUS
CN 4,7:14,17-Diimino-2,21-metheno-9,12-nitrilo-15H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 5-ethyl-10-[1-(heptyloxy)ethyl]-19-hexyl-16,18,19,20-tetrahydro-6,11,15,22-tetramethyl-18,20-dioxo-, methyl ester, (15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:569737 HCAPLUS
DOCUMENT NUMBER: 125:275490
TITLE: Syntheses of stable bacteriochlorophyll-a derivatives as potential photosensitizers for photodynamic therapy

AUTHOR(S): Kozyrev, Andrei N.; Zheng, Gang; Zhu, Chunfeng; Dougherty, Thomas J.; Smith, Kevin M.; Pandey, Ravindra K.
CORPORATE SOURCE: Dep. Radiation Biol., Roswell Park Cancer Inst., Buffalo, NY, 14263, USA
SOURCE: Tetrahedron Letters (1996), 37(36), 6431-6434
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB New methods for conversion of unstable bacteriochlorophyll-a present in Rb. sphaeroides into stable bacteriochlorins are presented. Cyclic imide derivs. from related cyclic isoimide or amide analogs are obtained by intramol. base catalyzed cyclization. Most of the new bacteriochlorins have long wavelength absorptions in the range of 796-822 nm. In preliminary screening, the isoimide analogs have shown promising in vivo photosensitizing activity for the treatment of cancer by photodynamic therapy.

IT **182253-28-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of stable bacteriochlorins as potential photosensitizers for photodynamic therapy)

RN 182253-28-7 HCAPLUS
CN 9,12-Imino-2,21-metheno-7,4:14,17-dinitrilo-4H-pyrido[4,3-b]azacyclononadecine-16-propanoic acid, 10-acetyl-5-ethyl-19-hexyl-1,5,6,15,16,18,19,20-octahydro-6,11,15,22-tetramethyl-18,20-dioxo-, propyl ester, (5R,6R,15S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.